

VICTORIA 2.0: A Mechanistic Model for Radionuclide Behavior in a Nuclear Reactor Coolant System Under Severe Accident Conditions

Prepared by
N.E. Bixler

Sandia National Laboratories

Prepared for
U.S. Nuclear Regulatory Commission



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Prepared by N. E. Bixler

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Sandia National Laboratories
Albuquerque, New Mexico 87185-0739

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Abstract

VICTORIA is a computer code that is intended to mechanistically treat fission product behavior and related phenomena in the reactor coolant system of commercial light water reactors. Processes that are treated by the VICTORIA models include the release of fission products and nonradioactive materials from fuel rods and degraded forms of fuel, the release of control rod elements and other structural materials, chemical interactions and change of phase, aerosol formation and interactions, transport and deposition of aerosols and vapors, resuspension of deposited aerosols, and decay heating effects due to transport and deposition of fission products. Excluded from this list are thermal hydraulics and most aspects of fuel degradation and relocation. It is possible to decouple these aspects of accident analysis from fission product behavior and transport because the coupling between these phenomena is primarily unidirectional, i.e., thermal hydraulics influence fission product behavior, but not vice versa.

VICTORIA provides the user with a detailed mass balance for each of the 26 elements that it treats. It also provides information on chemical speciation of vapors and condensed-phase materials. Finally, it provides a detailed description of the aerosols that remain suspended, of the quantities that deposit, and of the mechanisms that lead to deposition.

There are a number of new or improved features in VICTORIA 2.0. These include (1) improvements in the Booth model for fission product releases from fuel; (2) a new model, based on the Booth approach, for fission product releases from rubble beds; (3) a new option to treat three condensed phases; (4) a new model, based on Blackburn's model for UO_2 thermochemistry, for treating fuel oxidation, reduction, and volatilization; (5) new models for chemisorption of HI and I_2 onto oxidized metals; (6) a simple model for chemical kinetics at low temperatures; (7) a new model for aerosol deposition in a vena contracta; and (8) options to specify mass or molar flow rates instead of gas velocities.

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Executive Summary

Research during the 20 years since the reactor accident at Three Mile Island has led to significant advances in the state of knowledge of the key phenomena that govern the progress of a severe accident. Much of this knowledge has been codified into computer models that can be used to analyze hypothetical accident sequences and to evaluate safety issues. One such computer model is the VICTORIA code.

VICTORIA is intended to mechanistically treat fission product behavior and related phenomena in the reactor coolant system of commercial light water reactors, both pressurized water reactors and boiling water reactors, undergoing severe accidents. VICTORIA is also capable of analyzing the current generation of advanced light water reactors.

Processes that are treated by the VICTORIA models include the release of fission products and nonradioactive materials from fuel rods and degraded forms of fuel, the releases of control rod elements and other structural materials, chemical interactions and change of phase, aerosol formation and interactions, transport and deposition of aerosols and vapors, resuspension of deposited aerosols, and decay heating effects due to fission product transport and deposition. Excluded from this list are thermal hydraulics and most aspects of fuel degradation and relocation. It is possible to decouple these aspects of accident analysis from fission product behavior and transport because the coupling between these phenomena is primarily unidirectional, i.e., thermal hydraulics influence fission product behavior, but not vice versa.

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There are a number of new or improved features in VICTORIA 2.0, most of which resulted from the recommendations given by the VICTORIA Independent Peer Review Committee. These include (1) improvements in the Booth model for fission product releases from fuel; (2) a new model, based on the Booth approach, for fission product releases from rubble beds; (3) a new option to treat three condensed phases; (4) a new model, based on Blackburn's model for UO_2 thermochemistry, for treating fuel oxidation, reduction, and volatilization; (5) new models for chemisorption of HI and I_2 onto oxidized metals; (6) a simple model for chemical kinetics at low temperatures; (7) a new model for aerosol deposition in a vena contracta; and (8) options to specify mass or molar flow rates instead of gas velocities.

The structure of this manual has changed significantly from the previous version; it is now organized into four parts. Part I describes the theoretical bases and modeling approaches used in developing the code; Part II contains practical information for code users; Part III contains details of the databases used in the code; and Part IV describes the numerical methods. Part I contains five chapters. The first three of these are essen-

tial reading for the novice VICTORIA user. The last two chapters contain detailed descriptions of the modeling approaches used to treat chemistry and aerosol processes, and are intended for the more advanced user.

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The VICTORIA peer review committee has also contributed much to the current code version and to the format of this document. Members of this committee were V. Mubayi, D. R. Olander, J. Gieseke, and M. Schwarz. Recommendations made by this committee have guided and will continue to guide VICTORIA code development.

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Part I: Theoretical Bases and Modeling Approaches

1.0 Introduction and Overview

1.1 Phenomena in Severe Nuclear Reactor Accidents

The phenomena that govern the progression of a severe nuclear accident, such as the one at Three Mile Island (Rogovin, 1979), are extremely complex and, as a result, difficult to model. Early attempts to analyze the consequences of severe accidents in the Reactor Safety Study (WASH-1400, 1975) made overly conservative assumptions because many of the governing phenomena were not understood well enough to model accurately. Since then, a large body of research has been focused on understanding the key phenomena and codifying that understanding into computer models that can be used to analyze potential accident sequences. One such computer model is the VICTORIA code.

Severe accident sequences usually begin with some initiating event that leads to a reduction or halting of coolant flow through the core of the nuclear reactor, resulting in inadequate heat removal. Eventually, if coolant flow is not restored, the core begins to dry out and then to degrade. Rupture of the cladding often occurs in the vicinity of 1200 to 1300 K, depending on system pressure and on material interactions between the Zircaloy cladding and grid spacers, which have traditionally been fabricated from Inconel. Some release of fission products accompanies this early failure of the cladding; this early release is often referred to as the gap release, because most of this release is from fission products that have diffused into the gap or plenum regions of the fuel rods during normal operation. Diffusion of fission products in the fuel grains at temperatures in the vicinity of 1200 K is too slow to contribute much to the gap release (Matzke, 1986). The fission products that are released at this time are mostly the noble gases, iodine, and cesium.

The fuel cladding, the outer surface of which becomes lightly oxidized during normal operation, begins to oxidize rapidly when temperatures reach 1700 to 1800 K (Urbanic and Heidrick, 1978). Quite often oxidation is rapid enough that a flame front propagates through the fuel region. Most of the steam is converted to hydrogen at the flame front and the region above the front (assuming that the steam is flowing upward) is said to be steam starved. Cladding oxidation is highly exothermic, so fuel temperatures generally rise dramatically during this phase of the accident. Oxidized cladding is quite brittle and may crack and become permeable. Some of the unoxidized cladding, especially on the inner surface, may melt and interact with the fuel surface and/or relocate downward. Metallic Zircaloy in a steam-starved region can form hydrides. Interactions between coolant and Zircaloy cladding are primarily responsible for controlling the oxygen potential in the coolant during a severe accident, which in turn affects other phenomena, such as fission product chemistry. Fission product chemistry directly affects volatilities, which influence fission product release rates from fuel.

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In PWRs, the stainless steel control rod cladding generally fails at about 1700 K. Traditional control rods composed of silver/indium/cadmium alloy generate internal pressures of about 35 bar at the temperatures where the cladding fails, depending on the alloy composition. If system pressure is less than the internal pressure, control rod bursts can mechanically convert molten alloy into aerosols. Vaporization of control rod alloy also contributes to releases of the control rod elements. While control rod materials do not directly contribute much to severe accident consequences, they can alter the behavior of the fission products, and thus indirectly alter the consequences of a severe accident.

Under sufficiently oxidizing conditions and at high temperatures, volatilization of uranium from the fuel can be significant. Volatilization of uranium is a complicated phenomenon because several processes occur simultaneously. Oxygen must first diffuse to the surface of the fuel. There it can either react to modify the stoichiometry of the fuel (increase the excess oxygen in the fuel) or react to form UO_3 vapor, which is the most volatile uranium species under most accident conditions; however, other uranium vapors can form and contribute to the overall release. Like the control rod elements, uranium volatilization has little direct impact on the consequences of a severe accident, but it can serve to modify the behavior of released fission products and thus indirectly affect consequences.

During the phase in which the cladding is rapidly oxidized, the release of fission products into the coolant channel becomes much faster. The cladding deteriorates and becomes more permeable, the increased temperatures result in faster diffusion rates within the fuel grains and pores, and some of the fission product volatilities are greater in the steam-starved (hydrogen) environment above the flame front than they are in a steam-rich environment. Continued heating of the core by unremoved decay heat continues to enhance fission product release until significant changes in geometry begin to occur.

A number of factors can cause the fuel rods to convert to rubble. Excessive temperatures and fracturing during oxidation can cause the fuel cladding to lose mechanical strength and lead to collapse of a portion of the fuel rods. Fracturing can be significantly enhanced by the thermal shock caused during reflooding of the core, either due to accumulator injection or operator intervention. Thermal shock of the embrittled cladding can cause rapid conversion of a significant portion of the fuel rods to a rubble bed. Formation of a rubble bed usually reduces coolability, resulting in higher temperatures and, after a period of time, formation of a molten pool.

The molten pool may initially be held in place by an underlying, impermeable crust. Eventually, this crust and other supporting structures give way and the molten pool moves downward. The relocation process may ultimately lead to failure of the lower head and ejection of a portion of the core and internal structures onto the concrete basemat below the reactor vessel. This ejection can be pressurized or unpressurized, depending on the size and location of a previous failure in the primary coolant system or on the success of any operator intervention to depressurize the system. During the period of rubble and molten pool formation, fission products continue to evolve from the fuel. By the time

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a rubble bed is formed, most of the volatile fission products have been released. Less volatile fission product elements, such as barium, strontium, molybdenum, ruthenium, and possibly cerium and lanthanum, begin to evolve in larger quantity during this phase than the earlier phase of an accident. Uranium volatilization from a rubble bed can also be significant.

After failure of the lower head, a pathway exists for air to intrude into the reactor vessel. If an accident were to proceed to this point, oxygen partial pressures inside the core would increase suddenly and dramatically, and further oxidation of the Zircaloy and fuel would occur. This would result in a release of heat comparable to, or possibly greater than, that during the rapid oxidation of the cladding in steam. Some fission product volatilities, primarily molybdenum and ruthenium, would be enhanced under these highly oxidizing conditions. Little is known at present about the potential for release of fission products during this phase of an accident, although it is likely to be significant.

The thermal processes outlined in the preceding paragraphs induce natural convection within the reactor vessel and primary coolant system, as illustrated in Figure 1.1 for a pressurized water reactor (PWR). The source of heat during a severe reactor accident is, of course, decay heat from the fuel. However, after significant fission product release, some of this heat source has relocated from the core region to other points in the upper plenum and primary circuits. Heat sinks are primarily due to losses through surfaces. In some cases heat carried by coolant flows through a point of failure in the reactor coolant system (RCS) boundary may also be significant, especially during blowdown.

Natural convection patterns can be quite complex, in some cases involving three distinct zones of recirculation. One is in the core and upper plenum region, where flow is commonly downward near the relatively cool, outer wall and upward at the relatively hot, central portion of the core. A countercurrent flow can also set up between the upper plenum and steam generator inlet plena, with the hotter steam flowing toward the steam generator inlet plena through the top portion of the hot legs, and cooler steam flowing toward the upper plenum through the bottom portion of the hot legs. The third recirculation zone is through the steam generator tubes, where a portion of the tubes are involved in forward flow (toward the steam generator outlet plena) and the remainder are involved in backward flow (toward the steam generator inlet plena). The large surface area represented by the steam generator tubes makes this region an effective heat sink.

Fluid flows have a significant influence on the mass transport of fission products during a severe accident. Analyses of flow must consider both natural and forced convection, as indicated above. Thus, it is essential to treat heat transfer and fluid flow as coupled processes. The study of heat transport and flow phenomena in a nuclear reactor is commonly referred to as thermal hydraulics. In most cases, thermal hydraulics can be effectively decoupled from fission product behavior. Possible feedback mechanisms are clogging of flow paths by aerosol deposition and relocation of sources of decay heat.

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These feedback mechanisms have been found to be weak in all severe accidents investigated to date (Bixler, 1997).

Transport of fission products through and out of the RCS depends strongly on coolant flow patterns. Mass transport is also directly affected by the volatilities of the fission products, which determine whether they will be present as vapors or aerosols. Aerosol transport is strongly influenced by aerosol size distribution, which is in turn governed by processes that affect nucleation, growth, agglomeration, and deposition. Aerosols present during a severe accident are generally mixtures of liquid and solid (Mubayi et al., 1997). Some of the aerosols deposit onto surfaces, forming films that are two-phase mixtures. While deposited aerosols can be mechanically resuspended during periods of sudden flow increase, little is known at present about resuspension of partially molten films. Also, aerosol deposition under complex flow conditions and in nonsimple geometries is not well understood at present. However, aerosol deposition is understood well enough to adequately predict deposition in severe accident studies performed by the author.

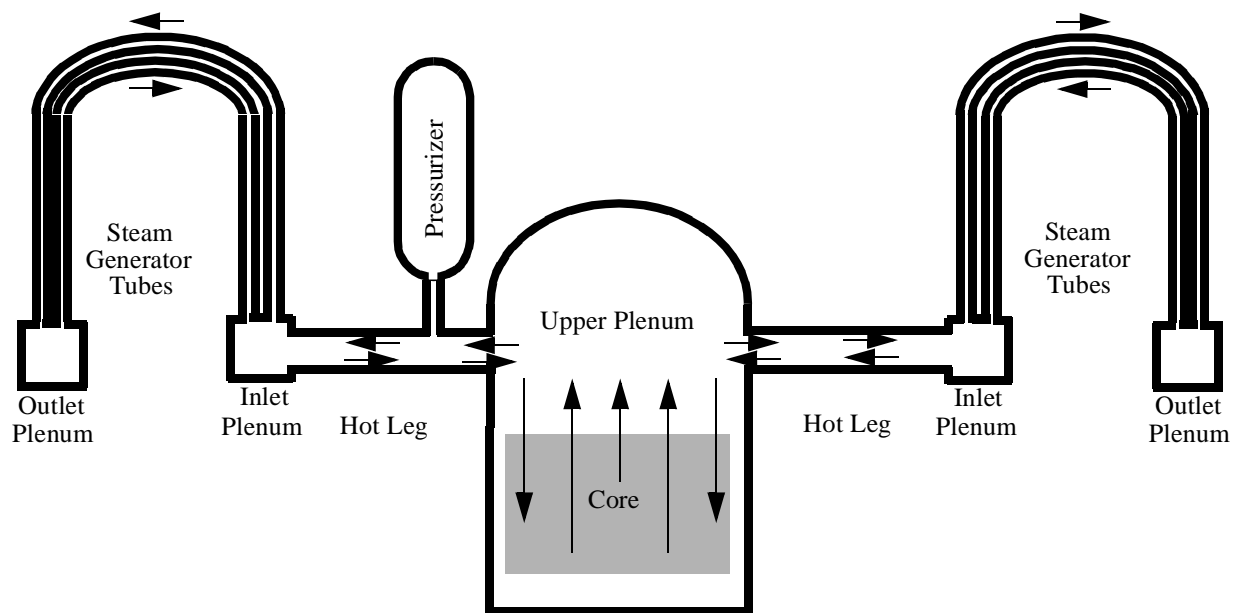


Figure 1.1. Schematic of plant with two primary circuits.

An important aspect of fission product behavior, which has only been alluded to in the preceding discussion, is chemistry. Chemistry governs volatilities, and so directly influences every other phenomenon affecting release and transport of fission products. Important chemical interactions in severe accidents include interactions among vapors, change of phase resulting in aerosol nucleation and growth or vapor condensation onto surfaces, chemical interactions between vapors and surfaces, and interactions among

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condensed-phase species on surfaces. Vapor-phase interactions include interactions between volatile fission products, steam, hydrogen, boron, and control rod elements. A change of phase can be congruent, such as vaporization of CsI, or incongruent, such as volatilization of UO_{2+x} to form UO_3 vapor. Interactions between vapors and surfaces include chemisorption, solution of hydrogen in metals, and oxidation of Zircaloy. Interactions between condensed phase species include interactions of condensed-phase fission-product species with uranium oxides to form uranates, and interactions to form eutectics, such as UO_2 interactions with ZrO_2 .

The study of possible chemical interactions during a severe accident is a challenging, almost formidable task. In part, this challenge is due to the almost endless list of species that could form. Sorting through this list of possible species requires some guidance from lab-scale experiments and larger-scale tests intended to simulate severe accidents. Compounding this challenge are the potentials for nonideal solution behavior and for chemical kinetics to limit the approach to equilibrium. Fortunately, very few chemical processes of importance during severe accidents are limited by chemical kinetics, at least at temperatures above 1000 K. At present, nonideal solution behavior has been studied for only a limited number of fairly simple chemical systems. While nonideal solution behavior may be important, establishing a defensible model for the highly complex chemical systems that affect fission product behavior during severe accidents is beyond current capabilities, except for a few cases. Thus, chemical equilibria and ideal solution treatments are the most reasonable framework upon which to build a model for fission product behavior in the RCS of a nuclear plant during a severe accident.

1.2 Intentions and Purpose of the VICTORIA 2.0 Code

VICTORIA is intended to mechanistically treat fission product behavior and related phenomena in the RCS of commercial light water reactors, both pressurized water reactors and boiling water reactors (BWRs), undergoing severe accidents. VICTORIA is also capable of analyzing the current generation of advanced light water reactors.

Mechanistic treatments of fission product behavior include models for release of fission products and nonradioactive materials from fuel rods and degraded forms of fuel, release of control rod elements and other structural materials, chemical interactions and change of phase, aerosol formation and interactions, transport and deposition of aerosols and vapors, resuspension of deposited aerosols, and decay heating effects due to fission product transport and deposition. Excluded from this list are thermal hydraulics and most aspects of fuel degradation and relocation. As mentioned, it is possible to decouple these aspects of accident analysis from fission product behavior and transport because the coupling between these phenomena is primarily unidirectional. While VICTORIA could be used to model aerosol processes in containment, some containment phenomena, such as removal of aerosols by sprays and effects of steam condensation on aerosol deposition, are not modeled. Thus, VICTORIA's capability to analyze fission product behavior in containment is somewhat limited.

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While the primary purpose for VICTORIA is to model severe accidents in commercial power plants, it is also essential that it be able to model small- and midscale experiments that are either separate effects or integral in nature. This secondary purpose is essential in order to assess and validate the models in VICTORIA. Assessment and validation are fundamental for developing and refining models, and ultimately for building confidence that the models are adequate for treating severe accident phenomena in commercial power plants.

Because VICTORIA is a mechanistic code, it is intended to be useful for understanding phenomena that, by necessity, are treated in a more empirical fashion in systems-level codes like MELCOR (Gauntt et al., 1998). Thus, VICTORIA should be useful for benchmarking codes like MELCOR. Furthermore, it should be possible to distill the trends from VICTORIA predictions into simplified models that can be used in the systems-level codes.

The VICTORIA code is not intended to be as fast running as other, less mechanistic codes. Nonetheless, CPU times must be reasonable and, in many cases, compromises between mechanistic modeling and CPU requirements have been made. The aim is that VICTORIA run quickly enough that sensitivity studies can be conducted, even for relatively complex plant studies. By and large, this aim has been accomplished, partially because of choices made in model implementation and partially because of the very powerful computers that are currently available.

The accuracy of the models in VICTORIA is limited much more by uncertainties in the underlying database than by the numerical implementation of the models. One of the largest sources of uncertainty comes from the Gibbs free energies that are used to determine thermochemical equilibria. The uncertainty in the equilibrium partial pressure of a vapor species can easily be a factor of 2 or more. While this uncertainty may seem large, it only corresponds to a temperature uncertainty of about 10 K. This level of uncertainty has been used as a yardstick for other modeling uncertainties. Individual uncertainties that do not appreciably increase the overall uncertainty of predicted releases receive a low priority when it comes to modeling improvements; those that appreciably increase the overall uncertainty of predicted releases receive a high priority.

1.3 New Features in VICTORIA 2.0

VICTORIA 2.0 contains a number of new or improved models, many of which resulted from the recommendations of the recently completed independent peer review (Mubayi et al., 1997). The following list briefly describes the most important of these new or improved models and references the sections of this manual where further details can be found:

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1. The Booth model for fission product diffusion in fuel grains now uses a “scaled time,” which accounts for variations in grain diffusivities with time. This model is described in Subsection 2.1.1.
2. A new model, based on the Booth approach, is available to treat fission product release from rubble beds, as described in Section 2.2.
3. A new option to treat three condensed phases (as opposed to a single condensed phase, as in previous versions of the code) has been added. This option is discussed in Subsection 4.1.3.
4. A new model, based on Blackburn’s model for uranium thermochemistry, can be used to treat uranium oxidation/reduction and volatilization. This model is described in Section 2.5 and Subsection 4.1.4.
5. VICTORIA 2.0 contains new models for chemisorption of hydrogen iodide and molecular iodine, as described in Subsection 4.2.2.
6. An option to treat chemical kinetics in a simplistic fashion is available, as discussed in Section 4.2.3.
7. A model for deposition in a vena contracta has been included in VICTORIA 2.0, as described in Subsection 5.6.5. This model can be used for flows from large, open regions into pipes, such as from an upper plenum into a hot leg.
8. Options to specify mass or molar flow rates instead of gas velocities have been added, as described in Subsection 6.5.3.
9. An option to enable subdomain coupling has been added, as described in Subsection 6.5.6. This option simplifies the process of subdividing a domain (a mathematical representation of a physical region such as a reactor vessel and coolant system) into subdomains, so that separate VICTORIA calculations can be performed on each subdomain.

Because of these improvements and other minor modifications to the VICTORIA code, input files developed for previous code versions are not compatible with VICTORIA 2.0; however, only minor modifications are required to convert input files to VICTORIA 2.0 format. Input file format is described in Chapter 6.

1.4 Overview of the VICTORIA Code

The structure of VICTORIA 2.0 is very similar to that of the previous version, VICTORIA 92-01 (Heames et al., 1992). The most important aspects of the code are described in this section in overview fashion. Details are presented in the subsequent chapters of this report.

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1.4.1 Nodalization

The finite difference nodalization used in VICTORIA is based on an axisymmetric coordinate system, although flow areas between nodes can be arbitrarily defined in the input file. The problem domain can be nodalized with up to 30 nodes in the axial dimension and up to 4 nodes in the radial dimension. Fuel rods are further subnodalized, with up to 2 subnodes, oriented radially, to represent the fuel pellets and additional subnodes to represent the fuel/clad gap and the fuel cladding. These concepts are clarified in the following examples.

Examples of VICTORIA nodalizations are shown in Figures 1.2 through 1.6. Figure 1.2 shows a simple nodalization that has been used to analyze many of the Oak Ridge National Laboratory (ORNL) horizontal induction (HI) and vertical Induction (VI) tests (Osborne and Lorentz, 1992) and the Sandia National Laboratories (SNL) source term (ST) tests (Allen et al., 1988, 1991). These tests were separate effects investigations of fission product release from spent fuel. Because the fuel from which the fission products were released was nearly isothermal in all of these tests, a single node is used in the VICTORIA representation of the experiments, as shown in Figure 1.2. This figure illustrates the subnodalization of the fuel rod: two nodes to represent the fuel pellets, a node to represent the gap, and a node to represent the cladding. Coolant flows in the axial direction, entering the domain from the bottom and exiting through the top. The coolant carries with it the fission products that are released from the fuel. Fission product transport within the fuel is primarily in the radial direction.

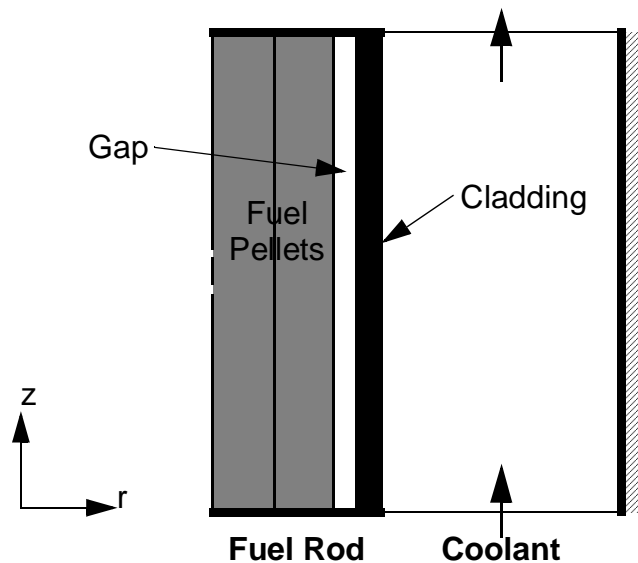


Figure 1.2. Illustration of nodalization used to analyze fission product release tests.

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Figure 1.3 illustrates the relatively simple nodalization used to represent the Falcon international standard problem (ISP) tests that were performed at Winfrith Technology Centre (Williams, 1994). VICTORIA was used to analyze the thermal gradient tube portion of the test apparatus, where many of the fission products condense and deposit. This was a “separate effects” test to evaluate capabilities to treat fission product chemistry and aerosol behavior. The VICTORIA nodalization corresponds to the post-test sectioning and chemical analyses that were performed so that data and predictions could be directly compared. Flow is axially from left to right.

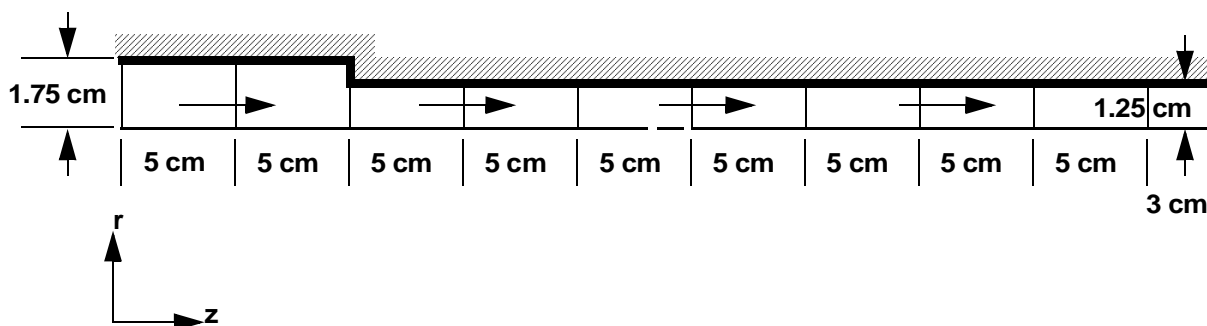


Figure 1.3. Illustration of nodalization used for Falcon ISP.

Figure 1.4 illustrates the nodalization used to represent the Phebus FPT-1 fuel bundle. In this case, both axial and radial temperature gradients existed throughout the duration of the test. Five axial nodes and two radial nodes (a total of ten) were used to represent the thermal gradients. The size of each node was chosen in order to achieve relatively uniform jumps in temperature from node to node. The flow was primarily axial during this test, as illustrated in the figure. The FPT-1 test used twenty 1-m long fuel rods and a single control rod; these fuel and control rods are not depicted in the illustration.

Figure 1.5 shows the 14-node representation used to analyze the Phebus FPT-1 circuit. A single radial node represents the 2- to 3-cm diameter pipe and fourteen axial nodes represent the length of the pipe. Note that while this pipe does not conform to a simple axisymmetric coordinate system, the coordinate system can be thought of as being deformed to follow the central axis of the pipe. This concept of a deformed coordinate system is commonly employed in VICTORIA analyses. Aerosol deposition in pipe bends is modeled through the use of flags, as described in Chapter 6.

Because fission product deposition was the major focus of this analysis, the nodalization was designed to achieve approximately uniform deposition on a per node basis. Some trial and error may be needed to obtain the same magnitude of deposition in each node. Furthermore, the choice of nodalization may be different, depending on whether the focus is on a single fission product, such as iodine; several fission products, such as

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iodine, cesium, and tellurium; or on all fission products. Nonetheless, achieving uniform deposition per node is a good criteria for choosing a nodalization when fission product deposition is the focus of the analysis.

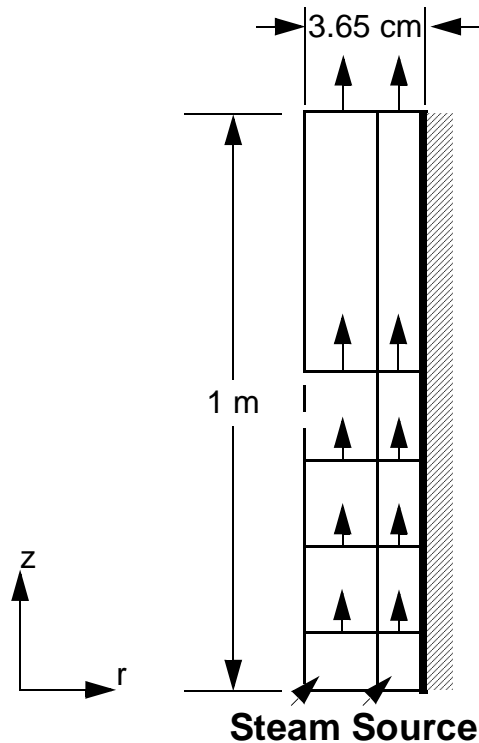


Figure 1.4. Illustration of 10-node representation of the Phebus FPT-1 fuel bundle.

Finally, Figure 1.6 illustrates a nodalization that was used to analyze a three-loop PWR (Bixler, 1997). This nodalization corresponds to the schematic shown in Figure 1.1. Only two loops are shown in the figures because one of the loops (the one on the left) used in the analysis actually represents two loops of the plant; this simplification was possible because the thermal hydraulics of two of the loops were essentially identical. On the other hand, the thermal hydraulics of the third loop (the one on the right) were quite different than those of the other two loops. This nodalization is quite complex compared with those in the previous illustrations. This figure shows that with some creativity, highly complex configurations can be represented with VICTORIA.

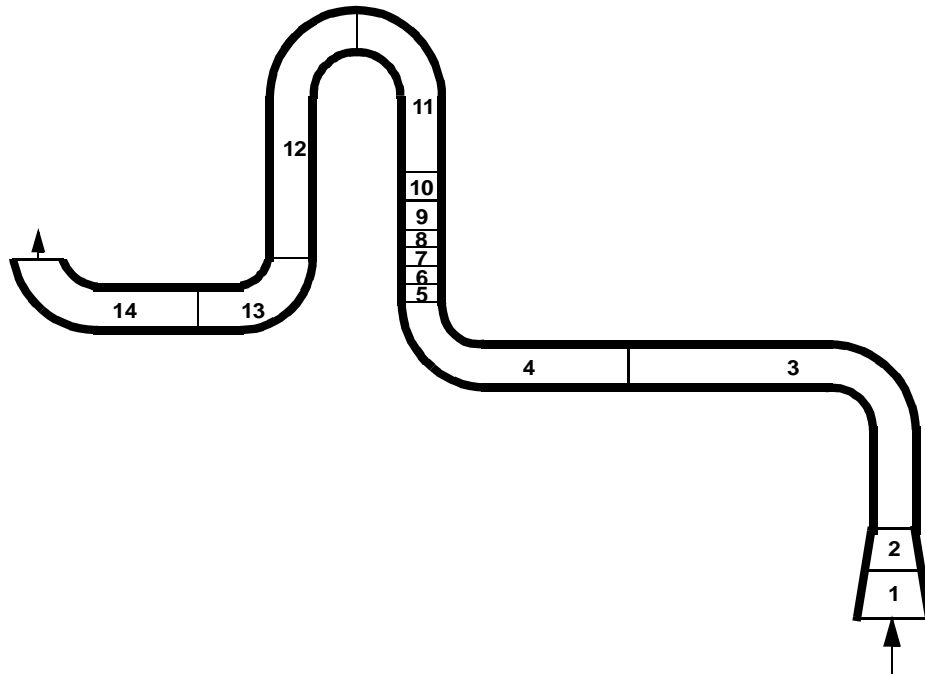


Figure 1.5. Illustration of nodalization used to analyze the Phebus FPT-1 circuit.

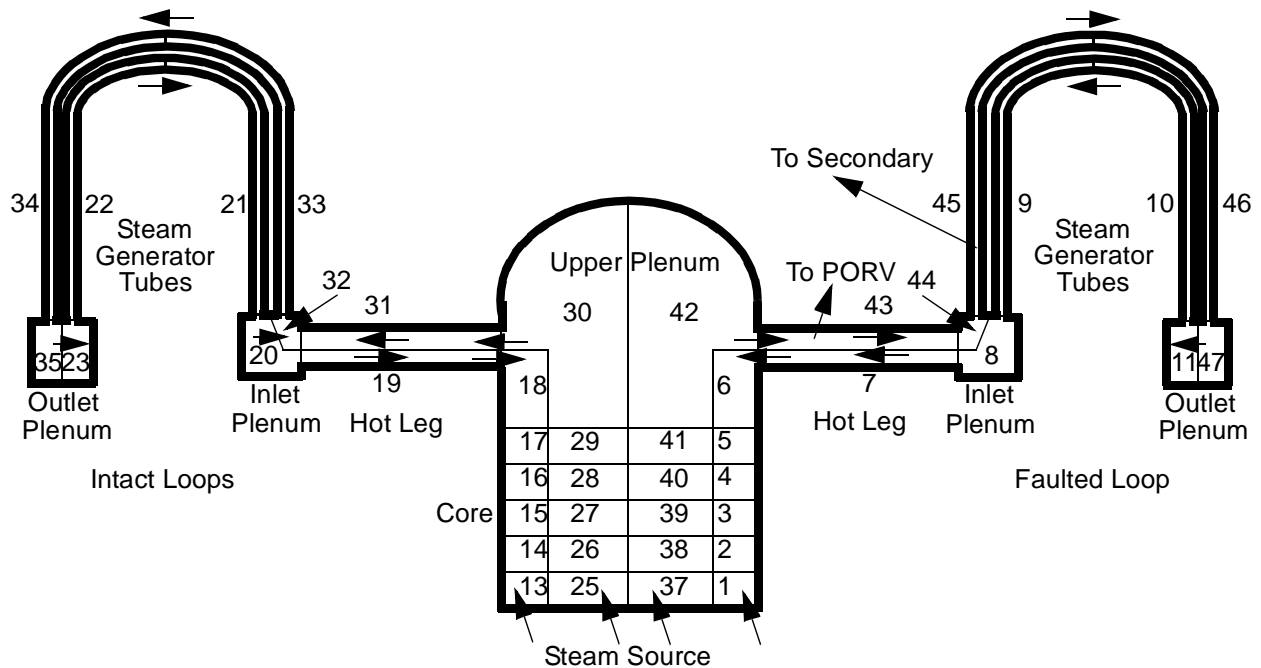


Figure 1.6. Illustration of a nodalization used to analyze the plant shown in Figure 1.1.

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1.4.2 Release of Fission Products from Fuel

The previous version of VICTORIA contained two options for analyzing fission product release from fuel rods. The two methods were based on the work of Booth (1957) and of Rest and Zawadzki (1992). In the peer review of the VICTORIA code (Mubayi et al., 1997), it was concluded that the Rest and Zawadzki model is too complex and contains too many poorly understood parameters to be useful as a predictive tool in a code such as VICTORIA and that this modeling option should be abandoned. As a result, VICTORIA 2.0 contains only the Booth modeling option for fission product release.

The implementation of the Booth model in VICTORIA is not entirely conventional. While the Booth model in its usual form is used to represent diffusion of fission products from the fuel grains to the interconnected pores, a porous media model is used to represent diffusion and Darcy flow of fission products through the pores, gap, cladding, and into the coolant channel. This implementation implies that overall release rates from fuel are dependent on total gas pressure. Other models, such as the various CORSOR models, do not account for any pressure dependence of fission product releases. Furthermore, experimental evidence to confirm a pressure dependence of fission product release rates is scant. While the theoretical underpinnings of the current fission product release model are sound, corroborative evidence is needed to confirm the relationship between pressure and release rates.

The Booth model in VICTORIA 2.0 has been extended to treat fission product release from rubble beds. This is a simple extension in which rubble beds are treated as unclad fuel rods. A model for fission product release from molten pools is lacking in VICTORIA 2.0. Current thinking is that fission product release from molten pools is very slow because of the low surface area between the molten pool and the coolant. Furthermore, the more volatile fission products are generally released well before a molten pool would form. Thus, the lack of a molten pool model in VICTORIA 2.0 is not a significant deficiency.

Release of the silver/indium/cadmium control rod alloy is modeled in the same way as in previous versions of VICTORIA. A burst release is modeled when internal pressure exceeds external pressure. The slower process of alloy vaporization is always modeled.

Improved models for fuel oxidation/reduction and uranium volatilization are included in VICTORIA 2.0. These models are based on Blackburn's formulation for the thermochemistry of UO_{2+x} (Blackburn, 1973), with the Green and Leibowitz correction (Green and Leibowitz, 1981). This model has been implemented at present for hyperstoichiometric fuel, i.e., $x > 0$; it will be implemented in a future version for hypostoichiometric fuel, i.e., $x < 0$. The current limitation to hyperstoichiometric fuel is very mild since it is highly unlikely that fuel would be reduced below UO_2 during a reactor accident. (However, such reduction could occur in some small-scale separate-effects tests performed in pure hydrogen or a hydrogen/inert gas mixture.)

1.4.3 Transport Within the Reactor Coolant System

No significant changes have been made in the treatment of fission product transport since the previous release of VICTORIA. While the independent peer review committee recommended that the explicit treatment of subregions (previously called films), which contain vapors and materials that have condensed or deposited onto a surface, be investigated and possibly eliminated (Mubayi et al., 1997), modeling of these subregions has been retained in VICTORIA 2.0. An investigation of these subregions indicates that the uncertainties in predictions arising from uncertainties in the thickness of these subregions are tolerable for most analyses; they are certainly much smaller than the uncertainties in equilibrium vapor pressures caused by uncertainties in the thermochemical database.

Modeling of the transport of vapor species accounts for advection and diffusion between nodes and diffusion within a node between the bulk gas and surfaces, including fuel rods, control rods, and mechanical structures. A Sherwood correlation that was an option in the previous version of VICTORIA has now been made the default, as recommended by the independent peer review committee (Mubayi et al., 1997). Aerosols are advected along with the gases, but may nucleate, grow, agglomerate, and deposit as well. Aerosol processes are discussed further in Subsection 1.4.5 below.

Fission product transport results in the relocation of a portion of the decay power from the core to the upper plenum and the primary circuits. The decay heating from deposited and suspended fission products in these regions can cause structures to heat up. Since the capability to treat decay heating of structures is lacking in codes that only perform thermal hydraulics calculations, this capability has been included in VICTORIA. While this is not a new model, it has proved to be essential for demonstrating that the feedback between fission product modeling and thermal-hydraulic modeling is generally very weak.

1.4.4 Chemical Processes

Treatment of chemical processes is largely the same as in previous versions of VICTORIA, with a few notable exceptions. Most chemical interactions are assumed to attain thermochemical equilibrium very quickly, which is a good assumption when temperatures are above 1000 K. Fuel chemistry is also taken to be at equilibrium; however, fuel pellet UO_2 thermochemistry is treated differently than in previous versions of VICTORIA. Blackburn's model for the equilibrium between fuel and oxygen (Blackburn, 1973), with the Green and Leibowitz correction (Green and Leibowitz, 1981), has been incorporated into VICTORIA 2.0, as recommended by the peer review committee (Mubayi et al., 1997). This model provides a more realistic approach to fuel oxidation and reduction, and to fuel volatilization. Furthermore, it regulates oxygen potential in the fuel pores, which in turn affects fission product chemistry.

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At the recommendation of the independent peer review committee, an option to treat three condensed phases has been added to VICTORIA 2.0. Using this option results in higher predicted volatilities than the single-phase option, which was the only choice in previous versions of VICTORIA. Increased volatilities generally result in earlier predicted releases from the fuel and less retention in the reactor coolant system.

The Urbanic and Heidrick (1978) correlation continues as the model for cladding oxidation. The peer review committee recommended that a more mechanistic approach to zirconium oxidation be included in the code. This may be considered for a later code release.

Several new models for chemisorption of fission product species onto structural materials are available in VICTORIA 2.0. In particular, chemisorption of hydrogen iodide and molecular iodine onto stainless steel surfaces can be modeled as an option.

A "frozen chemistry" model is new for VICTORIA 2.0. This model is a simple treatment of chemical kinetics. With this model, chemical interactions beyond simple change of phase are precluded below a user-specified threshold temperature. This model is implemented as an option.

Vaporization of control rod alloy is treated exactly as it was in previous versions of VICTORIA. However, the user is allowed more control over the quantity of alloy available for evaporation.

1.4.5 Aerosol Processes

Aerosol processes are treated in exactly the same manner as in previous versions of the code. The only addition to is a model to treat deposition in a vena contracta.

The aerosol models are based on the CHARM code developed by Wheatley (1988). Heterogeneous aerosol nucleation, growth, agglomeration, deposition, and mechanical resuspension are all treated. Aerosol nucleation is modeled by assuming that new particles have the minimum size allowed in the distribution. This is equivalent to modeling heterogeneous nucleation onto seed particles of a specified size. Aerosol growth is treated using the Fuchs-Sutugin growth law, as described in Hidy and Brock (1971).

Four agglomeration mechanisms are modeled. These are Brownian diffusion, gravitational settling, turbulent shear, and turbulent inertia. Each of these mechanisms can induce velocity gradients, which can cause aerosol particles to collide and agglomerate. Agglomeration terms are summed using the Saffman and Turner convention (1956).

Five aerosol deposition mechanisms are modeled. These include gravitational settling, deposition in a turbulent flow field, diffusion, thermophoresis, and flow irregularities. Deposition caused by five types of flow irregularities is considered: 90° pipe bends, abrupt contractions, upcomer-type cyclone steam separators, chevron-type steam dryers, and

vena contractas. A linear summation convention is used to determine a net deposition velocity.

The resuspension model in VICTORIA is based on data from the ORNL ART facility. This model is for dry-dust resuspension and does not account for differences in adhesion between aerosols and substrates. Because this model is not applicable in all situations, it has been made optional in VICTORIA 2.0, as recommended by the independent peer review committee (Mubayi et al., 1997).

1.5 Organization of the Report

This report is structured differently than earlier versions of the VICTORIA user's manual (Heames et al., 1990, 1992). It contains four parts: Part I, Theoretical Bases and Modeling Approaches; Part II, Users Guide; Part III, Thermochemical and Thermophysical Databases; and Part IV, Numerical Methods.

Part I contains five chapters. Chapter 1 presents background, an overview, and new features in VICTORIA 2.0. Chapters 2 and 3 provide detailed descriptions of the modeling of fission product releases from fuel and of vapor and aerosol transport in the reactor vessel and coolant system. These chapters are essential reading, especially for the new VICTORIA user. Chapters 4 and 5 are for the more advanced VICTORIA user and for those who are particularly interested in a more detailed understanding of the theoretical framework of VICTORIA. These chapters are focused on chemical and aerosol processes, respectively.

Part II is a practical guide on how to use the VICTORIA code. It has two chapters, which describe VICTORIA input and output, respectively. The chapter on output not only describes readable (ASCII) output files, but also a binary graphics file that can be used for plotting. These chapters are essential reading for anyone interested in running the VICTORIA code.

Part III consists of a single chapter that describes the thermochemical and thermophysical databases used in VICTORIA. This chapter will occasionally be a useful reference for the VICTORIA user.

Part IV also consists of a single chapter, which describes the numerical algorithms used in VICTORIA. This chapter is not essential for the average user but will be useful to those interested in numerical techniques.

Most VICTORIA users, then, should read Chapters 1 through 3 in Part I, skip to Chapters 6 and 7 in Part II, then read other portions of this report as need or interest dictates.

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2.0 Releases from the Core

Important releases during a severe accident include fission products from fuel; uranium from fuel; the principal cladding elements, zirconium and tin, from fuel cladding; and control rod elements, silver, indium, and cadmium. Releases from boron carbide control rods or blades are not currently treated. Examination of such releases was recommended by the peer review committee (Mubayi et al., 1997) and will be investigated in the future.

While releases of nonradioactive elements are of minor direct consequence, they can have a significant influence on fission product behavior and so must be treated in the model. The following sections discuss the models in VICTORIA for each type of release.

2.1 Fission Product Release from Fuel Rods

A schematic of a fuel rod is shown in Figure 2.1. Important parts of the fuel rod are the fuel pellet, which has a total porosity of α , the gap, and the fuel cladding. Fuel pellets are usually fabricated with a total porosity of about 4 to 5%. Most commonly, a parameter known as “fraction of theoretical density” is reported for fuel rods; this parameter is just 1 minus the total porosity.

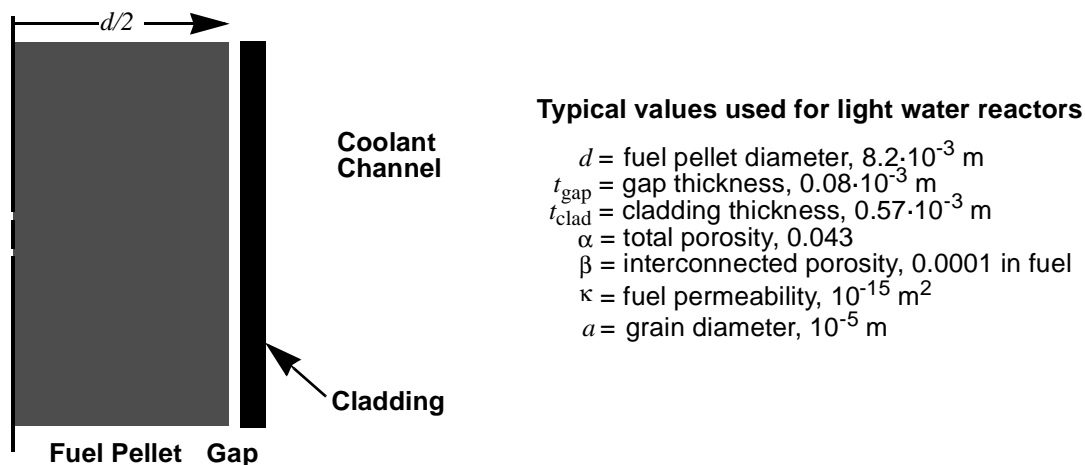


Figure 2.1. Schematic of a fuel rod and typical values used to describe fuel rod.

Fresh fuel is composed of nearly stoichiometric UO_2 , i.e., uranium and oxygen are present in a one-to-two molar ratio. The purpose of the fabricated porosity in the fuel pellets is to provide a place for fission gases, mostly the noble gases, xenon and krypton, to diffuse as they form from the fissioning of uranium during normal reactor operation. As fabricated, the interconnectivity of the pores is negligible. The fraction of the fuel that is

Releases from the Core

composed of interconnected pores is represented here by the Greek symbol β . As the burnup of the fuel increases, the porosity increases slightly and the interconnected porosity increases from negligible to about 0.0001. High burnup fuels may have even higher levels of interconnected porosity. Unfortunately, values of interconnected porosity have not been measured, so choices for this parameter are uncertain.

Surrounding the fuel is a void region called the gap. The purpose of the gap is primarily to allow for swelling of the fuel pellets, which occurs as the fuel burns up. The gap also provides an additional storage space for fission product gases after interconnected porosity becomes large enough to permit transport, and forms a pathway for gases to reach a plenum located at the top of the fuel rod. The gap and plenum are initially charged with helium at a specified pressure.

The fuel cladding, which is fabricated from Zircaloy, provides a boundary to prevent fission products from contaminating the coolant during normal operation. However, during a severe accident, the cladding becomes damaged, releasing fission products from the fuel into the coolant channel. Fuel cladding damage can occur from oxidation, rupture, or melting. VICTORIA treats cladding oxidation in a parametric fashion; rupture and melting occur when user-specified temperatures are reached.

Rupture of the fuel cladding usually occurs at a relatively low temperatures, 1200 to 1300 K. This process is generally initiated by swelling of the cladding and is accelerated by material interactions between cladding and grid spacers. (Rupture temperatures may be considerably higher in small-scale experiments where grid spacers are not present.) Clad rupture models are included in many of thermal-hydraulic codes (Allison et al., 1998; Gauntt et al., 1998). Information from these codes can be used to determine a clad failure temperature, which can then used as input to VICTORIA.

Melting of unoxidized Zircaloy occurs at about 2125 K; fully oxidized Zircaloy melts at almost 3000 K. The clad melting (relocation) temperature thus depends on the oxidation state of the cladding. On the other hand, fully oxidized cladding may not be able to retain its structural integrity and so may relocate at temperatures well below 3000 K. Again, information is usually extracted from a thermal-hydraulics code on the conditions for which cladding relocation occurs. This information is characterized as a clad melting temperature in the VICTORIA input.

At some point during the fuel degradation process, fuel rods degrade to debris beds. Conditions for this transition are usually obtained from thermal-hydraulics codes, many of which contain a semimechanistic or empirical treatment of this process (Allison et al., 1998; Gauntt et al., 1998). The formation of a debris bed is often triggered by rapid quenching of the fuel, which may be initiated by operator intervention or by accumulator injection. In either case, both cladding and fuel can be shattered by thermal stresses. Fission product release from a debris bed is discussed in Section 2.2.

Releases from the Core

Modeling of fission product release from fuel rods in VICTORIA is a sequential process involving five steps that are shown schematically in Figure 2.2. Important parameters for each step are also indicated in the figure. Fission products are assumed to be in the fuel grains at the start of an accident sequence. The first step is diffusion of the fission products from the interior of the grains to the grain surfaces. The model used is solid-state diffusion in a sphere and is based on the work of Booth (1957). This model is described in Subsection 2.1.1.

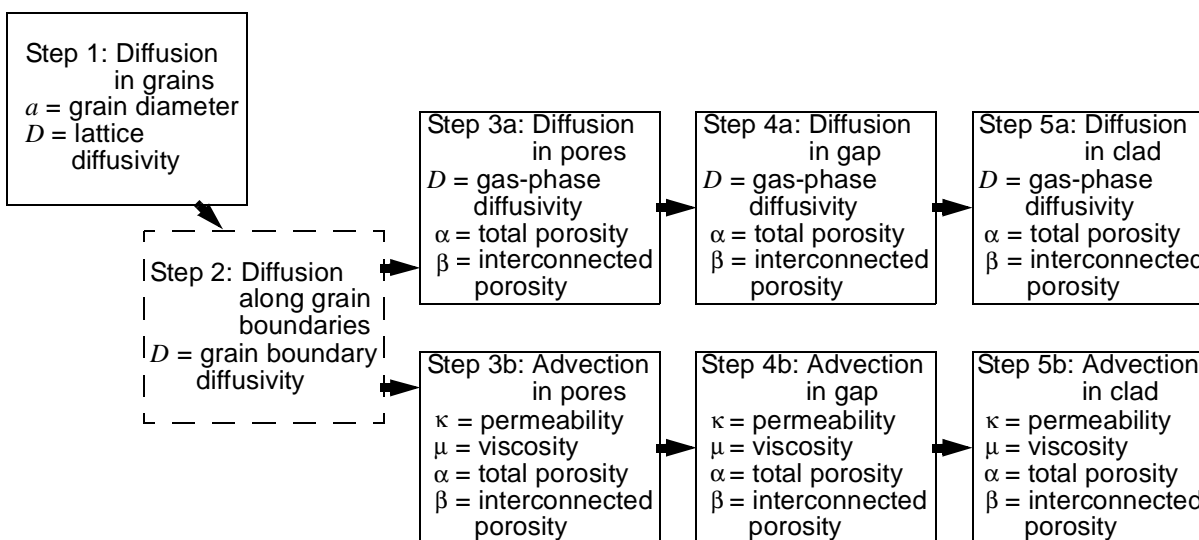


Figure 2.2. Fission product transport processes for release from fuel.

The second step, diffusion along grain boundaries to fuel pores, is assumed to be rapid and is not explicitly treated in VICTORIA. However, this step can be thought of as being subsumed in step 1. The grain diameter, a , used in the diffusion process does not have to be the true diameter of the grain. The modified diameter, often referred to as the “Booth diameter,” can account for other diffusion processes external to the grain. This concept was used by Booth in his original work, and others have followed this same line of reasoning. The assumption implicit in this line of reasoning is that other diffusion processes have a dependence on temperature similar to that of solid-state diffusion.

The third step is diffusion and advection through the pores to the external surfaces of the fuel pellets. This step is not modeled in other codes that treat fission product release from fuel, as far as the author knows. This step is important in the VICTORIA framework because only vapor-phase species can diffuse and advect within the fuel pellets; condensed-phase species remain on pore surfaces until conditions favor change of phase.

Releases from the Core

Thus, thermochemical equilibrium is brought into the release predictions in a natural way, i.e., by determining the volatility of each element, which depends on the species that form at the temperature and on the elemental compositions of the fuel pores. Other codes generally use a modified lattice diffusion coefficient that is intended to capture the effect of the volatility of the fission product elements. Unfortunately, this simple approach cannot capture the effects of oxygen partial pressure on release rates, or other chemical effects that affect speciation and volatility.

The treatment of diffusion also introduces another unique aspect of VICTORIA. The gas phase diffusion coefficients used in VICTORIA are inversely proportional to total gas pressure. As a result, release predictions are pressure dependent. Experimental data are scant concerning the pressure dependence of releases. Thus, the current modeling approach is based mainly on theoretical considerations. It is hoped that experimental data that can be used for validation or at least for confirmation of trends will be forthcoming from the VEGA tests being conducted in Japan. Validation of VICTORIA against such data was recommended by the VICTORIA Independent Peer Review Committee (Mubayi et al., 1997).

Steps 4 and 5 are similar to step 3, except that they take place in the gap and the cladding. These regions are also modeled as porous media. However, the porous structure in these regions may be entirely different than in the fuel pellets. For example, the gap is generally a thin annular region with total and interconnected porosities of unity. The permeability in this region should be approximately the same as that for loose sand, i.e., about 10^{-12} or 10^{-13} m², while the permeability of the fuel pellets should be several orders of magnitude lower, i.e., about 10^{-14} or 10^{-15} m². Unfortunately, there are no experimental data on which to base the value of fuel permeability; the choice of permeability for the fuel pellets and its effect on release modeling is discussed below.

As described earlier, the state of the fuel cladding evolves during a severe accident sequence. At the beginning of the accident, the cladding is intact and has neither interconnected porosity nor permeability. As long as the cladding remains intact, fission products can diffuse only as far as the inner cladding surface. Later in the sequence, the fuel cladding may rupture, oxidize, or melt; usually, a combination of these processes occurs. For example, the cladding may rupture at about 1250 K, oxidize autocatalytically at temperatures exceeding 1750 K, and melt at a temperature above 2125 K. As each of these phenomena occurs, the interconnected porosity and permeability of the cladding increases. These changes in the integrity of the cladding are modeled simplistically in VICTORIA, as described below.

Once fission products reach the outer cladding surface, they must diffuse to the bulk gas in the adjacent coolant channel. This diffusion process is the same as that at structural surfaces and is characterized by mass transfer through a boundary layer. This final step for fission product release is not shown in Figure 2.2 nor discussed in this chapter; it is discussed in Chapter 3.

2.1.1 Diffusion in the Fuel Grains

The mechanisms affecting release of fission products from fuel are thought to be quite complex (Olander, 1976), involving the formation and growth of bubbles, migration of bubbles, and grain boundary sweeping. While these processes can be modeled, the parameters affecting them are so numerous and so poorly understood that such models have little practical value for making quantitative predictions of fission product releases from fuel. The previous version of VICTORIA (Heames et al., 1992) contained such a model; however, it has been abandoned on the recommendation of the VICTORIA Independent Peer Review Committee (Mubayi et al., 1997). The somewhat less detailed but time-proven Booth model (Booth, 1957) has been retained as the sole option for predicting fission product releases from fuel rods.

In the Booth model, fission product transport occurs by simple diffusion in a spherical, solid-state region. As indicated, the spherical region more or less corresponds to a fuel grain. However, an effective diameter, greater than the grain diameter, may be used to account for diffusion processes external to the grain. This concept is retained in the VICTORIA framework to allow the user to account for fission product diffusion along grain boundaries, which is not treated explicitly. However, diffusion and advection processes in the interconnected fuel pores, gap, and cladding are treated separately and so are not represented in the Booth treatment, as implemented in VICTORIA. Assumptions in Booth's derivation are that diffusion coefficients and boundary conditions are constant. The mathematical expression of Booth's model is as follows:

$$\frac{\partial}{\partial t}C(i) = \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2D_G(i)\frac{\partial}{\partial r}C(i)\right] \quad (2.1)$$

subject to the following boundary conditions

$$C(i)|_{t=0} = C_G(0, i) \text{ for } 0 \leq r \leq a/2 \quad (2.2)$$

$$\frac{\partial}{\partial r}C(i)|_{r=0} = 0 \text{ for } t > t_0 \quad (2.3)$$

$$C(i)|_{r=a} = 0 \text{ for } t > t_0 \quad (2.4)$$

where

- t = time (s)
- r = radial coordinate (m)
- $C(i)$ = molar grain concentration of species i as a function of radius, r , and time, t
- $C_G(0, i)$ = uniform initial molar concentration of element i in the fuel grains (kg-mol/m³)
- $D_G(i)$ = grain lattice diffusion coefficient for element i (m²/s)

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a = actual or effective grain diameter (m)
 t_0 = initial time of calculation (s)

The basic result of Booth's work, modified to account for fission product solubilities in the lattice, is stated as follows:

$$\int_0^t S_G(i) dt' = [C_G(0, i) - C_S(i)] f(t, i) \quad (2.5)$$

where

$S_G(i)$ = fission product release rate of element i from the fuel grains into the fuel pores (kg-mol/m³·s)
 $C_S(i)$ = minimum of the solubility limit of fission product i in the fuel grains (kg-mol/m³) and the initial grain concentration, $C_G(0, i)$
 $f(t, i)$ = integral fraction of the initial inventory of fission product element i released at time t (dimensionless)

Currently, fission product solubilities in the fuel are treated as being negligible, with the exception of zirconium. The zirconium solubility in fuel is chosen to be 0.51 of the number of moles of uranium in the fuel (Kleykamp, 1993). This fraction is much greater than the initial inventory of zirconium in the fuel grains.

The solution for $f(t, i)$ is an infinite series, but Booth found that this series can be well approximated by the following expressions:

$$f(t, i) = 6 \left[\frac{\tau(i)}{\pi^3} \right]^{1/2} - 3 \frac{\tau(i)}{\pi^2} \text{ for } \tau(i) < 1 \quad (2.6)$$

and

$$f(t, i) = 1 - 6 \frac{\exp[-\tau(i)]}{\pi^2} \text{ for } \tau(i) \geq 1 \quad (2.7)$$

where τ is a scaled time that is defined as follows:

$$\tau(i) = \frac{\pi^2 D_G(i)(t - t_0)}{a^2} \quad (2.8)$$

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Equation (2.5) can be restated in a form that depends on current average grain concentration rather than initial grain concentration as follows:

$$\int_0^t S_G(i) dt' = [C_G(t, i) - C_S(i)] \frac{f(t, i)}{1 - f(t, i)} \quad (2.9)$$

This is the form that is actually used in VICTORIA.

The usual Arrhenius form is used to express the lattice diffusion coefficients as functions of temperature for each fission product element.

$$D_G(i) = D_0(i) \exp[-\theta(i)/T] \quad (2.10)$$

where

- $D_0(i)$ = preexponential coefficient for fission product element i (m^2/s)
- $\theta(i)$ = activation temperature of lattice diffusion for species i (K)
- T = absolute temperature (K)

Because D_G can vary with time (through time variation of the temperature, T) the assumption of constant lattice diffusivity made by Booth in his derivation does not apply. To overcome this shortcoming, the scaled time defined in Equation (2.8) is replaced with the following definition, as recommended by the peer review committee (Mubayi et al., 1997):

$$\tau(i) = \frac{\pi^2 \int_{t_0}^t D_L(i) dt'}{a^2} \quad (2.11)$$

Current recommendations for $D_0(i)$ and $\theta(i)$ are taken from Matzke (1986); these are $5 \cdot 10^{-5} \text{ m}^2/\text{s}$ and 45,000 K, respectively, for in-pile experiments and $5 \cdot 10^{-5} \text{ m}^2/\text{s}$ and 50,000 K, respectively, for both plant calculations and out-of-pile experiments. These recommendations are for release of the noble gases from moderate burnup fuels (20 to 40 GWd/MtU). Validation studies against Oak Ridge and Sandia National Laboratories fission product release data (Bixler et al., 1994) have shown that using Matzke's values for grain diffusion coefficients results in better agreement with the data than those obtained using the previously recommended grain diffusion coefficients from Oi and Takagi (1964, 1965).

In principle, lattice diffusion coefficients should be different for each fission product, i . Further work, based on recommendations from the peer review committee (Mubayi et al.,

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1997), may be performed to estimate improved values for lattice diffusion coefficients. For the time being, the recommended values can be used to make reasonable estimates of fission product releases, especially for the more volatile fission product elements.

2.1.2 Diffusion and Advection in the Fuel Pores

The governing equation for diffusion and advection of vapors through the fuel pores is

$$\alpha \frac{\partial}{\partial t} C(i) = \frac{1}{r} \frac{\partial}{\partial r} \left[r \beta D(i) \frac{\partial}{\partial r} C(i) - r C(i) u \right] + S_p(i) \quad (2.12)$$

where

- α = total porosity of the fuel (dimensionless)
- β = interconnected porosity of the fuel (dimensionless)
- r = radial coordinate (m)
- $D(i)$ = gas-phase diffusion coefficient for species i (m^2/s)
- u = radial component of superficial gas velocity (m/s)
- $S_p(i)$ = rate of vapor diffusion from grains into pores ($\text{kg-mol}/\text{m}^3$)

Initial and boundary conditions for Equation (2.12) are as follows:

$$C(i)|_{t=0} = C_0(i) \text{ for } 0 \leq r \leq d/2 \quad (2.13)$$

$$\frac{\partial}{\partial r} C(i)|_{r=0} = 0 \text{ for } t > t_0 \quad (2.14)$$

$$C(i)|_{r=d/2-\epsilon} = C(i)|_{r=d/2+\epsilon} \text{ for } t > t_0 \quad (2.15)$$

where

- $C_0(i)$ = initial molar concentration of species i ($\text{kg-mol}/\text{m}^3$)
- t_0 = initial time of calculation (s)
- ϵ = an infinitesimal quantity

Equation (2.15) is an expression of the continuity of fission product concentrations at the outer surface of the fuel pellets. The rate of vapors entering the fuel pores, $S_p(i)$, is determined by the rate at which fission products diffuse from the grains, $S_G(i)$, and by the volatility of the species that are calculated to exist in the fuel pores, as discussed in Chapter 4. For simplicity, β is described here as being the interconnected porosity of the fuel; for those acquainted with modeling of porous media, β can be thought of as being the interconnected porosity divided by the tortuosity of the fuel pellets.

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As indicated, direct measurements of β are unavailable. Current defaults used in the VICTORIA code are largely based upon validation experience by the code developers (Bixler et al., 1994). Due to uncertainties in these default values, they can be modified by the user, who may have access to proprietary data or may want to investigate the sensitivity of predictions to this uncertainty. Default values used for β are discussed below.

The gas-phase diffusion coefficient for a multicomponent mixture is constructed from binary diffusion coefficients, which are calculated from Chapman-Enskog kinetic theory (Bird et al., 1960). For each binary system, the binary diffusion coefficient, $D(i,j)$, is calculated using

$$D(i,j) = \frac{0.018824 \sqrt{T^3 \left(\frac{1}{M(i)} + \frac{1}{M(j)} \right)}}{P \sigma_{ij} \Omega_{D,ij}} \quad (2.16)$$

$$\sigma_{ij} = \frac{1}{2}(\sigma_i + \sigma_j) \quad (2.17)$$

$$\Omega_{D,ij} = \sqrt{\epsilon_i \epsilon_j} \quad (2.18)$$

where

- $D(i,j)$ = binary diffusion coefficient of gaseous species i diffusing through gaseous species j (m^2/s)
- $M(i)$ = molecular mass of species i ($\text{kg}/\text{kg-mol}$)
- P = total gas pressure (Pa)
- σ_{ij} = characteristic diameter for collisions between species i and j (\AA)
- σ_i = Lennard-Jones parameter for characteristic diameter of species i (\AA)
- $\Omega_{D,ij}$ = collision integral for mass diffusion in a binary mixture of i and j (dimensionless)
- ϵ_i = Lennard-Jones parameter for characteristic energy of self-interaction for species i (dimensionless)

Values for the Lennard-Jones parameters used in VICTORIA are found in Part III of this manual.

The following equation from Bird et al. (1960) is used to determine the diffusion coefficient for species i in a multicomponent mixture:

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$$\frac{1 - x(i)}{D_m(i)} = \sum_{\substack{j \in G \\ i \neq j}} \frac{x(j)}{D(i,j)} \quad (2.19)$$

where

- $x(i)$ = mole fraction of species i in the gas phase (dimensionless)
- G = the set of gaseous species in the VICTORIA database
- $D_m(i)$ = the diffusion coefficient of gaseous species i in the mixture of all other gaseous species (m^2/s)

There are two options available in VICTORIA for calculating gas-phase diffusion coefficients. In the first option, the diffusion coefficients are calculated assuming that there are only trace quantities of the fission products in a mixture dominated by steam, hydrogen, and helium. In this approximate representation, the summation in Equation (2.19) is only over these three species. In the second option, all gas-phase species in the VICTORIA database are considered in the summation; however, contributions from species that have a mole fraction less than 0.001 are considered to be negligible in order to reduce computational time. In either case, $D_m(i)$ from Equation (2.19) defines the value of $D(i)$ in Equation (2.12).

The radial component of velocity in Equation (2.12), u , is defined from Darcy's law to be

$$u = -\frac{\kappa}{\mu} \frac{\partial P}{\partial r} \quad (2.20)$$

where

- κ = permeability (m^2)
- μ = dynamic viscosity of the gas-phase mixture ($\text{kg}/\text{m}\cdot\text{s}$)
- P = total gas pressure (Pa), which is calculated in the fuel region by summing the partial pressures of the gas-phase species, i.e.,

$$P = \sum_{i \in G} p(i) \quad (2.21)$$

where

- $p(i)$ = partial pressure of species i (Pa)

Permeability varies according to the following relationship:

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$$\kappa(t) = \kappa_0 \frac{\beta(t)}{\beta_0} \quad (2.22)$$

where the subscript 0 indicates the initial value. The interconnected porosity, β , can increase if fuel frothing occurs during the accident sequence. The relationships used in VICTORIA to define interconnected porosity in the fuel pellets are as follows:

$$\beta = \beta_0 \text{ when } T \leq T_{fr} \text{ or } c(\text{H}_2) < c(\text{H}_2\text{O}) \quad (2.23)$$

$$\beta = \beta_0 + \beta_{fr} \left(\frac{T - T_{fr}}{200} \right) \text{ when } T_{fr} < T < T_{fr} + 200 \text{ and } c(\text{H}_2) \geq c(\text{H}_2\text{O}) \quad (2.24)$$

$$\beta = \beta_0 + \beta_{fr} \text{ when } T \geq T_{fr} + 200 \text{ and } c(\text{H}_2) \geq c(\text{H}_2\text{O}) \quad (2.25)$$

where

T_{fr} = temperature at which fuel frothing begins (K) [2300]

$c(i)$ = mass concentration of gaseous species i (kg/m³)

β_0 = initial interconnected porosity of fuel (dimensionless) [0.0001]

β_{fr} = interconnected porosity of fully frothed fuel (dimensionless) [0.001]

Quantities in square brackets indicate the default values used in VICTORIA. The model for interconnected porosity outlined in Equations (2.23) through (2.25) is based on observations made at the time of the ACRS ST-1 test (Allen et al., 1991). This was the first test in which fuel frothing was observed. Fuel frothing occurs when fission product elements that accumulate at grain boundaries begin to liquefy, allowing fuel grains to slide relative to one another. The result is that the fuel pellets can swell from the excess pressure created by release of volatile fission products from the fuel grains. At the time of the ST-1 test, the belief was that the phenomenon of fuel frothing only occurs under reducing conditions. (The ST-1 test was performed in a hydrogen/inert environment. Previous Oak Ridge tests had been performed in steam environments.) The rationale was that reducing environments cause fission products at grain boundaries to be reduced to their metallic state, allowing liquefaction to occur at much lower temperatures than under oxidizing conditions. More recent observations indicate that fuel frothing may occur even under relatively oxidizing conditions, i.e., in nearly pure steam. Some reevaluation of the default values used in the VICTORIA model for fuel frothing may be worthwhile as additional data become available.

Dynamic viscosity in Equation (2.20) is also calculated from Chapman-Enskog kinetic theory (Bird et al., 1960). The following equation is used to determine the dynamic viscosity represented by each gas-phase species:

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$$\mu(i) = 2.6693 \cdot 10^{-6} \frac{\sqrt{M(i)T}}{\sigma_i^2 \Omega_{\mu,i}} \quad (2.26)$$

where

$\Omega_{\mu,i}$ = viscosity collision integral for species i (dimensionless)
 $\mu(i)$ = viscosity of pure species i at temperature T (kg/m·s)

Values used in VICTORIA for the viscosity collision integral are given in Part III of this manual.

Equation (2.26) is used for all gaseous species except steam, for which the Meyer correlation is used (Meyer et al., 1967).

$$\mu(\text{H}_2\text{O}) = 3.082 \cdot 10^{-6} \left(\frac{T}{75.7} - 1 \right) \quad (2.27)$$

The viscosity of the mixture used in Equation (2.20) is calculated using the Wilke semiempirical formula (Bird et al., 1960):

$$\mu = \sum_{i \in G} \frac{x(i)\mu(i)}{\sum_{j \in G} x(j)\Phi_{ij}} \quad (2.28)$$

where Φ_{ij} is a dimensionless parameter that is defined as follows:

$$\Phi_{ij} = \frac{1}{\sqrt{8}} \left[1 + \frac{M(i)}{M(j)} \right]^{-1/2} \left\{ 1 + \left[\frac{\mu(i)}{\mu(j)} \right]^{1/2} \left[\frac{M(j)}{M(i)} \right]^{1/4} \right\}^2 \quad (2.29)$$

Equations (2.12) through (2.29) form a complete description of the processes modeled by VICTORIA for transport of fission product gases from fuel pores to the gap between fuel pellets and cladding. Details of how these equations are treated numerically are given in Part IV of this manual.

2.1.3 Diffusion and Advection in the Gap

The description for diffusion and advection of fission products in the gap between the fuel pellets and the cladding is very similar to that described in the preceding subsection for the fuel pores; however, axial transport can be important in the gap. For example, if the fuel rod fails at a single elevation, fission products can transport through the gap from

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locations above or below the failure point. Usually, the gap is the conduit for this transport. Thus, Equation (2.12) becomes for the gap

$$\alpha \frac{\partial}{\partial t} C(i) = \frac{1}{r} \frac{\partial}{\partial r} \left[r \beta_r D(i) \frac{\partial}{\partial r} C(i) - r C(i) u \right] + \frac{\partial}{\partial z} \left[\beta_z D(i) \frac{\partial}{\partial z} C(i) - C(i) v \right] \quad (2.30)$$

where

- α = total porosity of the gap (dimensionless) [1]
- β_r = interconnected porosity of the gap in the radial dimension (dimensionless) [1]
- β_z = interconnected porosity of the gap in the axial dimension (dimensionless) [1]
- v = axial component of gas velocity (m/s)

Initial and boundary conditions for Equation (2.30) are as follows:

$$C(i)|_{t=t_0} = C_0(i) \text{ for } (d/2) \leq r \leq (d/2 + t_{\text{gap}}) \quad (2.31)$$

$$C(i)|_{r=d/2-\epsilon} = C(i)|_{r=d/2+\epsilon} \text{ for } t > t_0 \quad (2.32)$$

$$C(i)|_{r=d/2+t_{\text{gap}}-\epsilon} = C(i)|_{r=d/2+t_{\text{gap}}+\epsilon} \text{ for } t > t_0 \quad (2.33)$$

$$\frac{\partial}{\partial z} C(i)|_{z=0} = 0 \text{ for } t > t_0 \quad (2.34)$$

$$\frac{\partial}{\partial z} C(i)|_{z=L} = 0 \text{ for } t > t_0 \quad (2.35)$$

where

- L = length of a fuel rod (m)

The interconnected porosities in the gap, β_r and β_z , are considered to be constant in the VICTORIA model for fission product release. By default, these interconnected porosities are both equal to unity.

The components of gas velocity, u and v , are defined in the same way as u in Equation (2.20):

$$u = -\frac{\kappa_r \partial P}{\mu \partial r} \quad (2.36)$$

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$$v = -\frac{\kappa_z \partial P}{\mu \partial z} \quad (2.37)$$

except that the permeability can be anisotropic, i.e., it can have different values in the radial and axial directions, where

κ_r = radial component of the permeability tensor (m^2)

κ_z = axial component of the permeability tensor (m^2)

Off-diagonal terms in the permeability tensor are taken to be zero, i.e., a radial pressure gradient does not induce an axial flow or vice versa. Gas viscosities and diffusion coefficients in the gap region are defined in exactly the same way as for the fuel pores, as described in Subsection 2.1.2.

2.1.4 Diffusion and Advection in the Fuel Cladding

Modeling of fission product transport through the cladding is analogous to that in the fuel pores. Interconnected porosities are transient and depend, in this case, on the calculated state of the cladding. The following equations apply

$$\alpha \frac{\partial}{\partial t} C(i) = \frac{1}{r} \frac{\partial}{\partial r} \left[r \beta D(i) \frac{\partial}{\partial r} C(i) - r C(i) u \right] \quad (2.38)$$

$$C(i)|_{t=t_0} = C_0(i) \text{ for } (d/2 + t_{\text{gap}}) \leq r \leq (d/2 + t_{\text{gap}} + t_{\text{clad}}) \quad (2.39)$$

$$C(i)|_{r=d/2+t_{\text{gap}}-\epsilon} = C(i)|_{r=d/2+t_{\text{gap}}+\epsilon} \text{ for } t > t_0 \quad (2.40)$$

$$C(i)|_{r=d/2+t_{\text{gap}}+t_{\text{clad}}-\epsilon} = C(i)|_{r=d/2+t_{\text{gap}}+t_{\text{clad}}+\epsilon} \text{ for } t > t_0 \quad (2.41)$$

The interconnected porosity is defined as follows:

$$\beta_r = 0 \text{ if } T < T_{\text{fail}} \quad (2.42)$$

$$\beta_r = \beta_{\text{fail}} \text{ if } T_{\text{fail}} \leq T \leq T_{\text{melt}} \quad (2.43)$$

$$\beta_r = \max(\beta_r, \beta_{\text{ox}}) \text{ if } C(Zr) < 0.5 \quad (2.44)$$

$$\beta_r = \beta_{\text{melt}} \text{ if } T \geq T_{\text{melt}} \quad (2.45)$$

where

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T_{fail}	=	temperature at which cladding is predicted to fail, e.g., by balloon rupture (K)
β_{fail}	=	interconnected porosity upon failure of the cladding (dimensionless) [1]
T_{melt}	=	melting temperature of the cladding (K)
β_{melt}	=	interconnected porosity upon melting of the cladding, usually unity (dimensionless) [1]
β_{ox}	=	interconnected porosity upon excessive oxidation of the cladding (dimensionless)

VICTORIA does not reset the interconnected porosity upon oxidation if the cladding has already failed (provided that $\beta_{\text{ox}} < \beta_{\text{fail}}$, which is normally the case). Most of the parameters affecting degradation of the cladding must be specified or at least can be modified in the VICTORIA input data. User control of these parameters is provided because VICTORIA does not contain a mechanistic model for cladding failure. Many thermal-hydraulic codes, such as MELCOR 1.8.4 (Gauntt et al. 1998), SCDAP/RELAP5 (Allison et al., 1998), and others, treat cladding failure in a mechanistic or empirical manner. Predictions from these codes can be used to control cladding failure in the VICTORIA model by selecting appropriate failure and melting temperatures.

2.2 Fission Product Release from Debris Beds

VICTORIA contains a simple debris bed model in which the debris bed is treated as a set of unclad cylinders. A debris bed can be the initial configuration for a calculation or can be formed during a calculation at the point when the cladding reaches its melting point. When the initial configuration is a debris bed, the pellet diameter can be chosen to reflect the diameter or surface-to-volume ratio of the debris particles; when cladding is lost as a result of increasing temperature, the particle diameter must be the value assigned to the fuel pellets because this dimension cannot be changed during a calculation.

Limitations to the current modeling of a debris bed are that particles are modeled as cylinders (spheres might better approximate the shapes of debris particles), particle diameters must be identical to fuel pellet diameters when the debris bed forms during a calculation, and mass transport from the particles to the bulk gas is not calculated appropriately for a debris bed when default parameters are used. However, the user can modify the default mass transport coefficients so the last limitation can be overcome. These limitations generally lead to slightly slower fission product releases from fuel than if the debris particles were treated in a more realistic fashion. Other aspects of the VICTORIA predictions, such as treatment of equilibrium chemistry, are independent of the actual fuel geometry.

With the exception of the gap and cladding, modeling of a debris bed is identical to that for a fuel rod, as described in Section 2.1. Fuel grains and fuel pores are modeled in the same way as discussed in Subsections 2.1.1 and 2.1.2. Fission products that reach the

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fuel particle surfaces then diffuse through a boundary layer into the bulk gas. This diffusion process is discussed in Chapter 3.

2.3 Fission Product Release from Molten Pools

VICTORIA does not contain a model for fission product release from molten pools at this time, but as explained above, this omission should have a relatively small effect on fission product releases from the core. The VICTORIA Independent Peer Review Committee recommended implementation of a simple molten pool model. In this model, fuel would melt gradually. The melting rate would be governed by the level of decay heat in the fuel at the time of melting. Using this model, the time required to completely melt the fuel in a node would be on the order of 10 minutes. The volatile fission products (noble gases, cesium, iodine, tellurium, and antimony) remaining in the fuel would be released in proportion to the fraction melted. Release of the other fission products would be treated as being mass transfer limited, with a highly reduced surface area for mass transfer between the molten pool and the bulk gas. The molten pool model recommended by the peer review committee may be implemented in a future code version.

2.4 Release of Control Rod Alloy

As mentioned above, release of control rod alloy has a negligible direct effect on the consequences of a severe accident; however, such releases may strongly affect fission product releases through chemical interactions (Chown and Williams, 1989). VICTORIA currently contains a model for release of silver/indium/cadmium alloy from control rods, but does not contain a model for release of boron carbide from control rods or blades. The peer review committee recommended that an option to model boron carbide releases be investigated (Mubayi et al., 1997). This recommendation could result in some future modeling enhancements.

The models employed in the VICTORIA code for release of the control rod elements have two parts: (1) a pressurized release, which converts control rod alloy directly to aerosols and (2) a slower vaporization process from alloy candling down the control rod cladding. These models are described in the following two subsections.

2.4.1 Burst Release

Control rod failure occurs when a portion of the control rod first reaches 1689 K. Once a control rod fails at a given elevation, it cannot fail at any other elevation because the internal pressure is relieved. The VICTORIA model for pressurization of a control rod is described in Chapter 4. Typically, internal pressure of a silver/indium/cadmium control rod at the failure temperature is about 3.5 MPa. If external pressure (total gas pressure in the coolant channel surrounding the control rod) is greater than or equal to the internal pressure at the time of control rod failure, then no burst release occurs; otherwise, if internal pressure exceeds external pressure, then a burst release occurs.

The VICTORIA model for a burst release from a control rod is based upon a set of small-scale experiments (Bowsher et al., 1986). Unfortunately, release data from a full-scale control rod are not available at this time; however, some useful information on control rod behavior could come out of the Phebus FP test series, which includes 1-m-long control rods. The data of Bowsher et al. indicate that about 2% of the alloy is converted into an aerosol, which has a log-normal size distribution, a geometric mean diameter of $0.5 \cdot 10^{-6}$ m, and a geometric standard deviation of 1.8. These parameters are used in the VICTORIA model for burst release with one qualification; only the portion of alloy above the level where control rod failure is predicted to occur is considered in the burst release. In addition to the formation of aerosols, the control rod vapors that exist just prior to failure are ejected into the bulk gas.

2.4.2 Alloy Vaporization

Two simple options are provided for treatment of vaporization of alloy following failure of a control rod. In the first option, which is the default, a film of specified thickness initially coats the surface of the control rod in each node at or below the failure point. This film neither drains nor is replenished and so a fixed mass of control rod alloy is available to vaporize over the balance of the calculation. The default film thickness is chosen to be $1.75 \cdot 10^{-4}$ m, but this value can be modified in the VICTORIA input.

In the second option, the film again has a specified initial thickness, but it is allowed to thin by drainage. A fluid mechanical treatment of the drainage of a film (Bird et al., 1960) indicates that the film thins as $1/\sqrt{t}$. In order to avoid a singularity at the point of control rod failure (i.e., when $t = 0$), an offset in time is used.

$$\delta_{CR}(t) = \delta_{CR}(0) \cdot \frac{\sqrt{t_o}}{\sqrt{t + t_o}} \quad (2.46)$$

where

- $\delta_{CR}(t)$ = thickness of the alloy film (m) as a function of time t , measured from the point of control rod failure
- $\delta_{CR}(0)$ = initial thickness of the alloy film (m)
- t_o = time offset (s) [10]

The value chosen as the default in the fixed film thickness option, $1.75 \cdot 10^{-4}$ m, is the thickness that would be attained if the initial film thickness were $1 \cdot 10^{-3}$ m after about 5 min. of drainage. From another perspective, $1.75 \cdot 10^{-4}$ m is approximately the average film thickness over a 20-min. period if the initial film thickness is $1 \cdot 10^{-3}$ m.

The models for vaporization of control rod elements are somewhat ad hoc. However, they are sufficiently flexible at present to mimic observed trends. Optionally, the user can

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prescribe releases of control rod elements as mass sources as a substitute for the models discussed in this subsection. Prescription of mass source data in the VICTORIA input is discussed in Part II of this manual.

2.5 Uranium Volatilization

Release of uranium by oxidative volatilization is treated as an equilibrium process. Details of the method used to compute the equilibrium between fuel and adjacent gases are given in Chapter 4. Uranium volatilizes from the outer surface of the fuel pellets directly into the fuel/clad gap. From there, it transports through the cladding to the bulk gas in the same manner as the fission products, as described in Subsections 2.1.3 and 2.1.4.

2.6 Release of Tin from Fuel Cladding

The current model for release of tin from fuel cladding assumes that significant tin release begins immediately after clad melting. The fraction of tin that can be released is equal to the fraction of zirconium that has oxidized; the remaining fraction of tin is removed along with the zirconium in which it is alloyed. Tin is assumed not to alloy with oxidized zirconium and so forms a separate metallic phase. This assumption is in keeping with the three-condensed-phase option discussed in Chapter 4. The fraction of tin associated with the oxidized portion of the zirconium is allowed to evaporate at a rate controlled by its vapor pressure (described in Section 4.3) and by mass transfer to the bulk gas (described in Section 3.3).

3.0 Fission Product Transport and Deposition

Fission product transport and deposition within the reactor vessel (RV) and reactor coolant system are governed by a number of complex processes. Modeling of fission product sources from the fuel is described in Chapter 2. Chemical equilibria among the released fission products and other materials, such as control rod alloy, determine speciation and govern the volatilities of the fission products. Species either condense directly onto structural surfaces or onto aerosol particles. While vapors that condense onto surfaces are immobile, as long as they do not revaporize, aerosol particles can be transported within and from the RCS. Of course, some of the aerosols deposit onto surfaces as well. All of these processes must be modeled to a reasonable degree of accuracy in order to determine the quantity and timing of fission products that are ultimately released to the atmosphere during a severe accident.

The focus of this chapter is on vapor and aerosol transport within the RV and RCS. This chapter also includes a discussion of decay heating of surfaces from deposited fission products. While modeling of chemical interactions and aerosol behavior enters the discussions in this chapter, the details of these models are covered in Chapters 4 and 5, respectively. The numerical aspects of the models used in VICTORIA are discussed in Part IV.

3.1 Modeling of Competitive Condensation

One aspect of modeling transport processes in the RV and RCS is connected with competitive condensation. Competitive revaporization is the converse of competitive condensation. While the discussion here is couched in terms of condensation, the concepts apply equally well to competitive revaporization.

When equilibrium conditions require that a vapor must condense (i.e., when its partial vapor pressure exceeds saturation) some of the vapor would normally condense onto structural surfaces and some onto aerosol particles. The competition for vapors to condense onto structures or onto aerosols is governed by mass transport. Vapors can diffuse from the gas to aerosol particle surfaces, which are usually assumed to be spherical, or they can diffuse to structural surfaces, which are assumed to be cylindrical in the VICTORIA representation. In either case, mass transport is governed by the diffusivity of the condensing vapor through the gas, by the surface area to which it is diffusing, and by the geometry of the surface. The situation is complicated by the fact that not all aerosol particles are the same size. If aerosols are graded by size, then each size class has its own geometrical properties, i.e., its own radius and total surface area. Mass transport does not occur at the same rate for each aerosol size class, so growth of the aerosols is not uniform across the size distribution.

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To complicate the picture even further, temperatures are often nonuniform within a node. In VICTORIA, the bulk gas is assumed to be isothermal, i.e., vapors and aerosols are at the same temperature. However, structural surfaces and the gases adjacent to those surfaces often have temperatures different than that of the bulk gas. This further affects the competition for condensation onto aerosol and structural surfaces because equilibrium vapor pressures at these surfaces are different. Simultaneous modeling of chemical equilibrium and mass transport in this rather complex system is not at all straightforward.

One approach—modeling vapors, aerosols, and structural surfaces as all being in equilibrium with each other—is not feasible because chemical equilibrium assumes thermal equilibrium, i.e., uniformity of temperature.

A second approach that might be used is to model vapors and aerosols as being in chemical and thermal equilibrium while structural surfaces are in chemical and thermal equilibrium with an infinitesimal layer of vapor adjacent to the surface. This second approach was the one recommended by the peer review committee (Mubayi et al., 1997). Unfortunately, this approach does not fit into the framework of the VICTORIA code for reasons that are better understood from the discussions in Chapter 4. In simple terms, the method for calculating chemical equilibrium in VICTORIA is based on a closed system, i.e., a fixed volume, fixed mass system. This method requires that there be a finite, not an infinitesimal, volume of vapor. The approach recommended by the peer review committee could best be implemented with an open chemical-equilibrium solver, in which the mass and composition of the condensed phase are fixed but the composition of the vapors is allowed to float. Such a solver would be open because the overall mass of each element in the system would not necessarily be conserved. While this recommendation is reasonable, it was not possible to implement it in time for the release of VICTORIA 2.0.

The approach used in VICTORIA 2.0, which is the one that was also used in previous versions, is to subdivide the entire region represented by a node into two, three, or four finite subregions, depending on whether fuel or control rods are present. Structural surface and bulk gas subregions must be present in each node. Chemical equilibrium is imposed on each of these subregions independently of the others. Each subregion has its own temperature, which may be different from the other subregions in the same node. With each subregion is also associated a volume, mass, and composition. Mass transfer among the three subregions is by diffusion and, in some cases, advection. This approach, which is retained in VICTORIA 2.0, is illustrated in Figure 3.1 for a node that contains a fuel rod and a structural surface.

One of the concerns of the peer review committee was that predictions might be sensitive to the thicknesses assigned to each of the subregions. The choices for these thicknesses affect the modeling of competitive condensation in the following way: (1) vapors that condense in the structural surface layer deposit directly onto the structural surface and (2) vapors that condense in the bulk gas region form aerosols. The default thick-

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nesses for the fuel, control rod, and structural layers are the diffusion boundary layer thicknesses, as described below. Sensitivity studies, in which these boundary layer thicknesses were varied from 0.2 to 5 times the default value (which the code developers believe to be an upper bound on the uncertainty of the competitive condensation mechanism), revealed an acceptable uncertainty in predictions for small-scale experiments (where surface-to-volume ratios are relatively large) and for plant-scale analyses (where surface-to-volume ratios are relatively small).

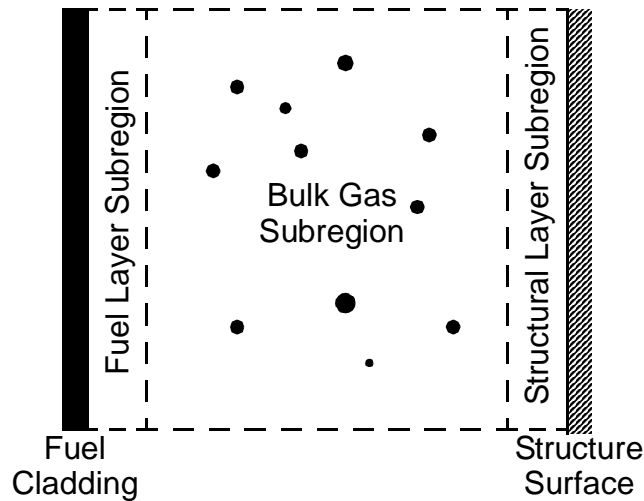


Figure 3.1. Illustration of subregions of a node employed in VICTORIA transport modeling.

3.2 Layer Thicknesses and Subregion Volumes

As mentioned earlier, diffusion boundary layer thicknesses are used as the default thicknesses for the fuel, control rod, and structural layer subregions. These thicknesses are calculated from a Sherwood correlation. However, in some cases geometric constraints require the subregion thickness to be less than the mass transfer boundary layer thickness, as explained below.

To construct the Sherwood correlation, first the Nusselt number for heat transfer is defined for various flow conditions as follows (Liles et al., 1988):

$$Nu = 4 \text{ when } Re < 2000 \quad (3.1)$$

$$Nu = 4 + 0.0099(Re - 2000) \text{ when } 2000 < Re < 3000 \quad (3.2)$$

$$Nu = 0.023Re^{0.8} \text{ when } Re > 3000 \quad (3.3)$$

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where

Re = Reynolds number (dimensionless), $(\rho U D_H)/\mu$

Nu = Nusselt number (dimensionless), $(h D_H)/k$

ρ = gas density (kg/m³)

U = gas speed (m/s), $\sqrt{u^2 + v^2}$

u = radial component of velocity (m/s)

v = axial component of velocity (m/s)

D_H = hydraulic diameter (m)

μ = dynamic viscosity (kg/m·s)

h = heat transfer coefficient (W/m²·K)

k = thermal conductivity (W/m·K)

Equation (3.2) is simply an interpolation between the ranges covered by (3.1) and (3.3). Equations (3.1) through (3.3) relate to forced convection, i.e., advection. Another set of correlations is used to determine whether natural convection may dominate advection. These are the following:

$$\text{Nu} = 0.59 \text{Ra}^{1/4} \text{ for } \text{Ra} < 10^9 \quad (3.4)$$

$$\text{Nu} = 0.1 \text{Ra}^{1/3} \text{ for } \text{Ra} > 10^9 \quad (3.5)$$

where

Ra = Rayleigh number (dimensionless), $(g|T_s - T_g|\rho^2 D_H^3)/(\mu^2 T_s)$

g = gravitational acceleration (m/s²)

T_s = surface temperature of fuel rod, control rod, or structure (K)

T_g = gas temperature (K)

VICTORIA uses the maximum of the Nusselt numbers for advection and convection in its treatment of mass transfer boundary layer thickness. Once the Nusselt number is defined for heat transfer, then the mass and heat transfer boundary layer thicknesses are defined as follows:

$$\delta_m = \delta_T = \frac{D_H}{\text{Nu}} \text{ when } \text{Nu} = 4 \quad (3.6)$$

$$\delta_m = \frac{\delta_T}{\text{Sc}^{1/3}} = \frac{D_H}{\text{NuSc}^{1/3}} \text{ when } \text{Nu} > 4 \quad (3.7)$$

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where

δ_m = mass transfer boundary layer thickness (m)

δ_T = heat transfer boundary layer thickness (m)

Sc = Schmidt number (dimensionless), $\mu/\rho D(i)$

The mass transfer boundary layer thicknesses from Equations (3.6) and (3.7) are used in the Section 3.3 to express mass transfer coefficients.

Geometric constraints impose maximum thicknesses for the subregions in order to maintain a finite volume in the bulk gas subregion. The volumes of the subregions must sum to the total volume of the node as follows:

$$V_N = V_B + V_F + V_C + V_S \quad (3.8)$$

where

V_N = volume of node (m³)

V_B = volume of bulk gas subregion (m³)

V_F = volume of fuel layer subregion (m³)

V_C = volume of control rod subregion (m³)

V_S = volume of structural layer subregion (m³)

The maximum thickness of the subregions is found by setting V_B to 0 in Equation (3.8). The default thickness for each of the subregions is then determined from the following equation:

$$\delta = \min(\delta_m, \delta_{\max}/2) \quad (3.9)$$

where

δ = subregion layer thickness (m)

δ_{\max} = maximum subregion layer thickness (m)

The user has several options for changing the default layer thicknesses, as explained in Part II of this report.

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3.3 Transport of Vapor-Phase Species

Transport of vapors within the RV and RCS is governed by an expression of the conservation of mass, which is stated for each species, i , as follows:

$$\frac{\partial}{\partial t}c(i) = \frac{1}{A_r}\frac{\partial}{\partial r}\left[A_r D(i)\frac{\partial}{\partial r}c(i) - A_r u c(i)\right] + \frac{1}{A_z}\frac{\partial}{\partial z}\left[A_z D(i)\frac{\partial}{\partial z}c(i) - A_z v c(i)\right] + \frac{S_F + S_C + S_S}{V_B} \quad (3.10)$$

subject to the following initial and boundary conditions:

$$c(i) = c_0(i) \text{ when } t = t_0 \quad (3.11)$$

$$\frac{\partial}{\partial t}c(i) = 0 \text{ on all domain boundaries} \quad (3.12)$$

where

- t = time (s)
- $c(i)$ = mass concentration of species i (kg/m³)
- r = radial coordinate (m)
- z = axial coordinate (m)
- A_r = area for flow and diffusion in radial dimension (m²)
- A_z = area for flow and diffusion in axial dimension (m²)
- $D(i)$ = diffusivity of species i in the gas mixture (m²/s)
- u = radial component of velocity (m/s)
- v = axial component of velocity (m/s)
- S_F = source of mass from fuel layer (kg/s)
- S_C = source of mass from control rod layer (kg/s)
- S_S = source of mass from structural surface layer (kg/s)
- V_B = volume of the bulk gas subregion (m³)
- 0 = subscript referring to initial condition

The diffusivities, $D(i)$, used in Equation (3.10) are calculated from Equations (2.16) through (2.19). The radial and axial velocity components, u and v , must be taken from a separate calculation or from experimental data. Mass source rates, S_F , S_C , and S_S , are calculated from the following relationships:

$$S_F = K_F(i)A_F[x_F(i) - x(i)] \quad (3.13)$$

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$$S_C = K_C(i)A_C[x_C(i) - x(i)] \quad (3.14)$$

$$S_S = K_S(i)A_S[x_S(i) - x(i)] \quad (3.15)$$

where

- $K(i)$ = mass transfer coefficient for species i ($\text{kg/m}^2\cdot\text{s}$)
- A = surface area for mass transfer (m^2)
- $x(i)$ = mole fraction of species i (dimensionless)
- F, C, S = subscripts to indicate fuel rod, control rod, and structure surface, respectively

When the fuel rod is clad, the mass transfer described by Equation (3.13) is at the external surface of the cladding; when the fuel rod is unclad, it is at the external surface of the fuel pellets. The numerical treatment of Equation (3.10) used in VICTORIA is described in Part IV of this report.

The mass transfer coefficients in Equations (3.13) through (3.15) are defined using the mass transfer boundary layer thicknesses from Equations (3.6) and (3.7) as follows:

$$K(i) = \frac{M(i)D(i)}{\delta_m} \sum_{j \in G} C(j) \quad (3.16)$$

where

- $M(i)$ = molecular mass of species i (kg/kg-mol)
- $C(j)$ = molar concentration of species j (kg-mol/m^3)
- G = set of gaseous species in the VICTORIA database

The Sherwood number (Sh) is a dimensionless number that characterizes mass transfer and is equivalent to the Nusselt number for heat transfer. The Sherwood number is defined as follows:

$$Sh = \frac{K(i)D_H}{M(i)D(i) \sum_{j \in G} C(j)} = \frac{D_H}{\delta_m} \quad (3.17)$$

Thus, Equations (3.13) through (3.15) can be rewritten in the form

$$S_F = \frac{ShM(i)D(i)}{D_H} A_F [C_F(i) - C(i)] = \frac{M(i)D(i)}{\delta_m} A_F [C_F(i) - C(i)] \quad (3.18)$$

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3.4 Condensation of Vapors onto Aerosol Surfaces

Equation (3.10) describes the transport of vapors through the domain of interest. For a plant analysis, the domain is usually the RV, the RCS, a secondary circuit, or some combination of these. For an analysis of an experiment, the domain can be any portion of the test apparatus. However, Equation (3.10) does not account for any chemical interactions of vapors. Possible interactions include the interaction of vapor species to form new vapor species, the condensation of vapor species to form the equivalent condensed-phase species, or an interaction of vapor species to form new condensed-phase species. Typically, all of these possibilities occur simultaneously. These interactions act as sources and sinks for each vapor species; however, these sources and sinks are not explicitly included in Equation (3.10) because chemistry is modeled as a separate step in VICTORIA, rather than simultaneously with vapor transport. Treatment of chemical interactions is discussed in Chapter 4 and the numerical aspects of this treatment are described in Part IV of this report.

While the total quantities of vapor- and condensed-phase species are determined by chemical interactions, the relative quantities of a species that condense onto each size class of aerosol is a matter of mass transport. As mentioned earlier, the arguments presented in this section are couched in terms of vapors that are condensing, but the arguments apply equally well when aerosols revaporize.

Modeling mass transport from a vapor phase to a single aerosol particle can be idealized as diffusion from an infinite vapor region to a spherical surface. By further assuming that the aerosol particle travels at the same velocity as the gas, the mathematical description of the problem is spherically symmetric. Simple theories exist for vapor diffusion in a continuum, which is relevant when the aerosol particle is much larger than the mean free path in the gas; and for free molecular diffusion, which is relevant when the particle is much smaller than the mean free path in the gas. However, in some cases the particle diameter is the same order as the mean free path of the gas molecules, and so neither of these theories applies. Fuchs and Sutugin (as reported in Hidy and Brock, 1971) worked out an approximate solution for the entire range of particle Knudsen numbers; this number is the ratio of the mean free path in the gas to the particle radius. Their solution is as follows:

$$\zeta(i) = 4\pi D(i) r_a [c_\infty(i) - c_a(i)] \left(\frac{1 + \text{Kn}}{1 + 1.71 \text{Kn} + 1.33 \text{Kn}^2} \right) \quad (3.19)$$

where

$\zeta(i)$ = the rate of condensation (evaporation is expressed by a negative value) of vapor species i onto the aerosol surface (kg/m^3)
 r_a = radius of the aerosol particle (m)

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- $c_{\infty}(i)$ = mass concentration of species i in the gas far from the aerosol particle (kg/m^3)
 $c_a(i)$ = mass concentration of species i in equilibrium with the surface of the aerosol particle (kg/m^3)
 Kn = particle Knudsen number (dimensionless)
= l_p/r_a
 l_p = mean free path of a gas molecule (m), which is calculated from

$$l_p = \mu \sqrt{\frac{\pi}{2P\rho}} \quad (3.20)$$

- P = total gas pressure (Pa)

In VICTORIA, Equation (3.19) is not used as an absolute rate for mass flux to an aerosol surface; rather, it is used to determine the relative rate of condensation onto particles of each aerosol size class. This is done in order to enforce thermochemical equilibrium within the bulk gas, i.e., change of phase is taken to occur instantaneously, but mass is transferred to each aerosol particle at the relative growth rate determined by (3.19).

A second process that causes aerosols to grow in size is agglomeration. Agglomeration occurs when aerosol particles collide and stick together. Agglomeration reduces the number of particles but increases their size. The mechanisms that cause agglomeration and the models for these mechanisms are discussed in Chapter 5.

3.5 Transport and Deposition of Aerosols

Aerosols are generally transported with the bulk gas, which moves with prescribed velocity, (u,v) . However, aerosol particles can move relative to the bulk gas and may deposit onto surfaces by several mechanisms. These mechanisms are described here in general terms; details are given in Chapter 5.

Gravitational settling may induce deposition onto upward-facing horizontal surfaces (floors). In some situations aerosol particles can grow to sufficient size that internodal settling can occur (e.g., settling velocities may exceed upward gas velocities) causing aerosol particles to fall from one node to another at a lower elevation. Thus, settling can result in deposition onto a surface, internodal settling, or a combination of both. VICTORIA models all of these possibilities.

The representation for aerosol velocities in VICTORIA is as follows:

$$v_a = v + F_g v_g \quad (3.21)$$

where

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- v_a = axial velocity component of aerosol particle (m/s)
- v = axial component of gas velocity (m/s)
- F_g = settling parameter, which can vary between -1 and +1 (dimensionless)
- v_g = particle settling velocity (m/s)

The purpose of the settling parameter is to define the orientation of gravity. The parameter is simply the cosine of the angle between the direction of gravitational acceleration and the z axis. When the z axis points upward, this parameter takes the value of -1.

Aerosols deposit onto surfaces when aerosol particle trajectories deviate from the gas streamlines. Deviation of aerosol particle trajectories from gas streamlines can lead to impaction of aerosols with surfaces. In many cases this impaction occurs because the aerosol particles are heavier and have more inertia than an equivalent volume of gas. Thus, aerosol particles may not be able to change direction as rapidly as gas particles. An example of this is in a pipe bend.

Five mechanisms for aerosol deposition onto surfaces are treated in VICTORIA. The first of these has already been described: settling. Aerosol particles only settle onto upward-facing surfaces; all other deposition mechanisms are independent of the orientation of the surface. The settling velocity used in VICTORIA incorporates Cunningham's slip correction (Cunningham, 1910), which accounts for noncontinuum effects for small particles.

The second deposition mechanism is connected with turbulent flow fields. Turbulent deposition occurs because of the chaotic nature of the flow field. Aerosol particles are unable to follow the same trajectories as the lighter gas particles; the result is that some of the particles collide with surfaces. Two separate models for turbulent deposition are used: one for submicron particles and another for supermicron particles. The two models are due to Davies (1966) and Sehmel (1970), respectively.

The third deposition mechanism is diffusion associated with Brownian motion of aerosol particles, which occurs when gas molecules collide randomly with aerosol particles. Diffusion of aerosol particles occurs under all flow conditions, but is easily dominated by other mechanisms, such as turbulent deposition. Diffusive deposition of aerosols is modeled in VICTORIA only when the flow field is laminar. The model used in VICTORIA is based on the work of Gormley and Kennedy (1949).

The fourth deposition mechanism modeled by VICTORIA is thermophoretic deposition, which occurs when there is a temperature difference between the bulk gas and the surface. Thermophoretic deposition was first reported by Tyndal (1870), who observed a dust-free zone surrounding a hot body. In a steady state and under the influence of a uniform temperature gradient, aerosol particles are observed to move with constant velocity toward the lower temperature. The thermophoretic force arises from collisions between the aerosol particles and the fluid molecules. Since the mean momentum transfer due to these collisions is proportional to the square of the gas temperature, a net force is

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exerted on the aerosol in the direction of the lower temperature region. The model for thermophoretic deposition used in VICTORIA is based on the work of Brock (1962).

The fifth deposition mechanism is aerosol impaction onto surfaces caused by flow irregularities. Five specific flow irregularities are modeled in VICTORIA. The first is deposition in 90° pipe bends. Depending on the size distribution of the aerosol particles, some are unable to negotiate the bend and impact the pipe surface on the outer, downstream portion of the bend (Pui et al., 1987). A second type of flow irregularity occurs in the vicinity of a sudden contraction in a pipe. Again, due to inertial effects, some aerosol particles collide with the pipe surface, mostly on the upstream side of the sudden contraction (Ye and Pui, 1990). The third type of flow irregularity occurs in steam separators. These exist on the primary side of a BWR and on the secondary side of a PWR. Steam separators set up a swirling flow, causing aerosol particles to be thrown toward the outer surface of the device. The fourth type of flow irregularity is in steam dryers. Again, these exist on the primary side of a BWR and on the secondary side of a PWR. These devices contain chevron-shaped guides with a number of bends that alternate in direction. Flows through steam separators and dryers in a PWR are typically too slow under severe accident conditions to induce any significant deposition because of the flow irregularities. Flows through these devices in a BWR are likely to be faster than in a PWR and might induce aerosol deposition under during severe accidents. The steam separator and dryer models used in VICTORIA are borrowed from the RAFT code (Im et al., 1987). The fifth type of flow irregularity is similar to the second, but it is the limiting case in which the upstream diameter is very large compared with the downstream diameter. Impaction of aerosol particles occurs because inertial effects prevent particles from making the turn as rapidly as the gas. A good example is the flow from the upper plenum of a reactor vessel into a hot leg. This type of flow is sometimes referred to as a vena contracta. The model used in VICTORIA is based on the work of Belyaev and Levin (1972). Guidance on when it is appropriate to use the sudden contraction and vena contract models is given in Chapter 5.

Aerosol deposition velocities from the five mechanisms described above are summed linearly to determine the net deposition velocity according to the following formulas:

$$u_c = -u_g + u_t + u_d + u_T \quad (3.22)$$

$$u_w = u_t + u_d + u_T + u_b \quad (3.23)$$

$$u_f = u_g + u_t + u_d + u_T \quad (3.24)$$

where

u_c = net deposition velocity at a ceiling surface (m/s)

u_w = net deposition velocity at a wall surface (m/s)

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u_f	=	net deposition velocity at a floor surface (m/s)
u_g	=	deposition velocity for gravitational settling (m/s)
u_t	=	deposition velocity in a turbulent flow field (m/s)
u_d	=	deposition velocity for diffusion in a laminar flow (m/s)
u_T	=	deposition velocity for thermophoresis (m/s)
u_b	=	deposition velocity induced by flow irregularities (m/s)

The deposition velocities depend on aerosol size. VICTORIA models the size distribution of aerosols in each node, as explained further in Chapter 5. Deposition velocities are calculated for each aerosol size. Net deposition rates are calculated by integrating over the size distribution.

Gravitational settling enhances deposition onto floors and diminishes that onto ceilings. Velocities induced by flow irregularities are always toward walls. Details of each of the deposition models, as well as other aspects of the aerosol modeling are provided in Chapter 5. Part IV of this report discusses numerical implementation of these models.

3.6 Radioactive Decay Heating

One consequence of the deposition of vapors and aerosols onto structural surfaces in the RCS during a severe accident is that radioactive decay of the deposited fission products may heat up those surfaces. This heatup may cause some of the deposited material to revaporize. Revaporization of deposited fission products is a chief concern during the late stages of an accident, especially if the containment has failed. It is also conceivable, although unlikely, that radioactive decay heating could lead to early failure of an RCS component and subsequent depressurization.

The VICTORIA models used to treat decay heating are described in this section. Decay powers are modeled for each of the fission product elements in the database. Data used for decay powers and for material properties are given in Part III of this report.

In principle, decay heating affects thermal hydraulics. The influence of decay heating on thermal hydraulics has been investigated for several accident sequences and so far has been found to be negligible. The current approach to performing VICTORIA analyses makes the assumption that coupling between thermal hydraulics and fission product behavior is nearly unidirectional, i.e., that fission product behavior depends strongly on thermal hydraulics, but thermal hydraulics are nearly independent of fission product behavior. At present, this assumption appears to be justified.

The model developed by Ostmeier (1984) is used here to describe radioactive decay heating. It is based on data for the decay heat per mass of each isotope (ANSI, 1979) and on data for the relative abundance of these isotopes during normal operation of a commercial reactor (Bennett, 1979). In this model, decay chains are treated by ascribing

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the power produced by a daughter element to the parent. This modeling approach is appropriate for VICTORIA, which does not treat individual isotopes or radioactive decay chains.

Ostmeyer's model exploits the fact that isotopic abundances of the more unstable isotopes, which produce most of the decay power, quickly reach a steady state during normal operation. Ostmeyer assumes that this steady state has been reached prior to a reactor scram, which occurs near the beginning of an accident. With these assumptions, the decay power produced by each element is a fraction of the operating power just before scram. This fraction is purely a function of time after scram.

This section describes the decay heating model employed in VICTORIA. A more detailed description is given in Bixler (1993).

3.6.1 Modeling Assumptions

Several simplifying assumptions are made in the derivation of the mathematical model for decay heating described below. The important assumptions are the following:

All isotopes of an element have the same diffusive and transport properties. Thus the relative abundances of isotopes are the same everywhere in the RCS.

Heat generated by gamma radiation is absorbed within the surface film. The peer review committee recommended that the fraction of gamma radiation that is absorbed locally be a user-prescribed parameter (Mubayi et al., 1997). Because this recommendation was assigned a low priority, it has not yet been implemented.

The temperature of the deposited film and underlying structure are characterized by a single temperature. Furthermore, the temperatures in these two regions are assumed to be quasi-steady.

The thermal properties of the deposited film, underlying structure, and any insulation surrounding the structure, are independent of temperature.

The ambient temperature surrounding the structure is constant.

Decay heat and the resulting heatup of structures produce an insignificant temperature rise in the gas.

Radiation losses are ignored.

The first assumption affects the calculation of decay power resulting from deposited fission products. The other assumptions affect the thermal response to decay heating.

3.6.2 Decay Power

Radioactive decay power is calculated from the following expression:

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$$Q = \delta_{\text{dep}} \sum_{j \in E} q(j, t) M(j) \sum_{i \in S} a_{ji} C(i) \quad (3.25)$$

where

- Q = decay power per unit surface area (W/m^2)
- δ_{dep} = thickness of the deposited film (m)
- $q(j, t)$ = decay power per mass of fission product element j as a function of time t (W/kg)
- $M(j)$ = molecular mass of element j (kg/kg-mol)
- a_{ij} = the number of moles of element j in 1 mole of species i (dimensionless)
- E = the set of elements in the VICTORIA database
- S = the set of species in the VICTORIA database

Here, the first summation is over the set of elements, j , and the second is over the set of species, i , in the VICTORIA database. The rate of heat generation by atomic fissioning per unit mass of element, j , is expressed by $q(j, t)$. Evaluation of $q(j, t)$ requires some normalization in order to account for the quantities of stable isotopes that have accumulated in the fuel, which depend on the burnup of the fuel. This is calculated from the total operating power of the reactor just prior to shutdown. The decay power for each isotope can then be calculated from a normalized power for each fission product element as follows:

$$q(j, t) = Q_{\text{Tot}} \tilde{q}(j, t) / m(j) \quad (3.26)$$

where

- Q_{Tot} = total operating power prior to reactor scram (W)
- $\tilde{q}(j, t)$ = the ratio of decay heat for fission product j to total operating power prior to scram as a function of time, t (dimensionless)
- $m(j)$ = inventory of fission product j in the fuel at the onset of the accident (kg)

Time in Equations (3.25) and (3.26) is measured relative to the time of scram.

3.6.3 Thermal Response of Structures

Ordinarily, VICTORIA does not compute temperatures, either for gases or for structures. However, because VICTORIA may get thermal-hydraulic input from codes that do not calculate fission product behavior, and so cannot determine decay heating in deposited films, a model for the thermal response of structures has been developed as part of the VICTORIA suite of models so that decay heating effects can be assessed. This subsection discusses the model for thermal response of structures that is employed in the VICTORIA code. The model is discussed in more detail in Bixler (1993).

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The governing equations for heatup of deposited films and the underlying structures are the following heat balances:

$$\delta_{\text{dep}} \rho_{\text{dep}} C_{P, \text{dep}} \frac{dT_{\text{dep}}}{dt} = Q - L_{dg} - L_{dS} \quad (3.27)$$

$$\delta_S \rho_S C_{P, S} \frac{dT_S}{dt} = L_{dS} - L_{SI} \quad (3.28)$$

which are subject to the following initial conditions:

$$T_{\text{dep}} = T_S = T_S(0) \text{ at } t = t_0 \quad (3.29)$$

where

- ρ_{dep} = density of deposited film (kg/m³)
- ρ_S = density of structure (kg/m³)
- $C_{P, \text{dep}}$ = heat capacity of deposited film (W/kg·K)
- $C_{P, S}$ = heat capacity of structure (W/kg·K)
- T_{dep} = temperature of deposited film (K)
- T_S = temperature of structure (K)
- $T_S(0)$ = initial temperature of structure (K)
- Q = decay power per unit surface area (W/m²)
- L_{dg} = heat flux from the deposited film to the gas (W/m²)
- L_{dS} = heat flux from the deposited film to the structure (W/m²)
- L_{SI} = heat flux from the structure to the insulation or thermal boundary layer surrounding the structure (W/m²)
- t_0 = initial time of calculation (s)

The heat flux terms are expressed using heat transfer coefficients as follows:

$$L_{dg} = h_{dg}(T_{\text{dep}} - T_g) \quad (3.30)$$

$$L_{dS} = h_{dS}(T_{\text{dep}} - T_S) \quad (3.31)$$

$$L_{SI} = h_{SI}(T_S - T_I) \quad (3.32)$$

where

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- h_{dg} = heat transfer coefficient between deposit and gas (W/m²·K)
 h_{dS} = heat transfer coefficient between deposit and structure (W/m²·K)
 h_{SI} = heat transfer coefficient between structure and insulation or gas surrounding structure (W/m²·K)
 T_g = gas temperature (K)
 T_I = outer surface temperature of insulation or ambient gas temperature outside of structure (K)

Heat transfer coefficients in VICTORIA are calculated for surfaces that are oriented normal to the radial or axial dimensions. The details of these calculations are given in Bixler (1993).

The solution of Equations (3.27) through (3.29) can be expressed analytically as follows:

$$T_{\text{dep}} = C_1 \exp(r_1 t) + C_2 \exp(r_2 t) + D_1 \quad (3.33)$$

$$T_{\text{dep}} = C_3 \exp(r_1 t) + C_4 \exp(r_2 t) + D_2 \quad (3.34)$$

where the coefficients r_1 , r_2 , C_1 , C_2 , C_3 , C_4 , D_1 , and D_2 have the following definitions:

$$r_1 = \frac{-(h'_1 + h'_2 + h''_2 + h'_3) + \sqrt{(h'_1 + h'_2 - h''_2 - h'_3)^2 + 4h'_2 h''_2}}{2} \quad (3.35)$$

$$r_2 = \frac{-(h'_1 + h'_2 + h''_2 + h'_3) - \sqrt{(h'_1 + h'_2 - h''_2 - h'_3)^2 + 4h'_2 h''_2}}{2} \quad (3.36)$$

$$h'_1 = \frac{h_1}{\delta_{\text{dep}} \rho_{\text{dep}} C_{P, \text{dep}}} \quad (3.37)$$

$$h'_2 = \frac{h_2}{\delta_{\text{dep}} \rho_{\text{dep}} C_{P, \text{dep}}} \quad (3.38)$$

$$h''_2 = \frac{h_2}{\delta_S \rho_S C_{P, S}} \quad (3.39)$$

$$h'_3 = \frac{h_3}{\delta_S \rho_S C_{P, S}} \quad (3.40)$$

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$$C_1 = \frac{h'_2(T_S - D_2) - (r_2 + h'_1 + h'_2)(T_{\text{dep}} - D_1)}{\sqrt{(h'_1 + h'_2 - h''_2 - h'_3)^2 + 4h'_2h''_2}} \quad (3.41)$$

$$C_2 = \frac{-h'_2(T_S - D_2) + (r_1 + h'_1 + h'_2)(T_{\text{dep}} - D_1)}{\sqrt{(h'_1 + h'_2 - h''_2 - h'_3)^2 + 4h'_2h''_2}} \quad (3.42)$$

$$C_3 = \frac{r_1 + h'_1 + h'_2}{h'_2} C_1 \quad (3.43)$$

$$C_4 = \frac{r_2 + h'_1 + h'_2}{h'_2} C_2 \quad (3.44)$$

$$D_1 = \frac{(h''_2 + h'_3)(Q' + h'_1 T_g) + h'_2 h'_3 T_I}{h'_1 h''_2 + h'_1 h'_3 + h'_2 h'_3} \quad (3.45)$$

$$D_2 = \frac{h''_2(Q' + h'_1 T_g) + (h'_1 + h'_2)h'_3 T_I}{h'_1 h''_2 + h'_1 h'_3 + h'_2 h'_3} \quad (3.46)$$

$$Q' = \frac{Q}{\delta_{\text{dep}} \rho_{\text{dep}} C_{P, \text{dep}}} \quad (3.47)$$

This analytical solution is used to determine the heatup of deposited films and the underlying structures. The gas temperature is assumed to be unaffected by decay heating effects.

The decay heat model in VICTORIA is optional and can be used in one of two modes. It can be used to simply determine the decay power in a deposited layer, or it can be used to adjust deposited film and structure temperatures. In either case, decay power data generated by VICTORIA could be used to augment the thermal-hydraulic analysis used to generate the input data for VICTORIA.

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4.0 Chemical Processes

A distinguishing feature of the VICTORIA code is that it treats chemistry in a much more detailed fashion than do any of the other severe accident codes, such as MELCOR (Gauntt et al., 1998). Chemistry has a profound effect on many of the processes that control fission product transport within and from the reactor coolant system. The effect is felt primarily through volatilities, which influence releases from fuel, aerosol behavior, and vapor condensation directly onto surfaces. Only the noble gases are immune to chemical interactions and remain as vapors under all the circumstances that would exist during a severe accident.

The chemical forms of iodine that would exist during a severe accident, and especially the dominant forms that would be released into containment under severe accident conditions, have been a topic of much debate (Silberberg, 1986). Early in the study of severe accidents, it was thought that most iodine entering containment would be in a vapor form (WASH-1400, 1975). These early concepts have made their way into current licensing regulations, resulting in some unnecessary and uneconomical operational procedures. Since then, additional research on iodine chemistry has been performed. This work has led to the view that most of the iodine entering a containment during a severe accident would be in aerosol rather than vapor form (Soffer et al., 1995).

Another issue where chemistry is critical relates to the later phases of a severe accident. In many cases, significant fractions of the fission products released from the core region would be retained in the RCS during the early phases of an accident. However, questions arise about the potential for the deposited material to be revaporized later in the sequence if RCS temperatures increase gradually or suddenly. The potential for revaporization of the deposited fission products depends on their chemical forms as well as their physical locations within the RCS. The VICTORIA code, with its comprehensive suite of chemical models, is a valuable tool for answering such questions.

The spectrum of chemical processes that could occur during a severe accident is extensive. Some chemical interactions are nonideal. Others are limited by mass transport kinetics, such as Zircaloy oxidation and the chemisorption of cesium onto oxidized Inconel or stainless steel. However, in most cases, chemical kinetics are rapid and the approach to equilibrium is well approximated as being instantaneous. This is generally true in regions where temperatures exceed 1000 K; at temperatures well below 1000 K, chemical kinetics may play a significant role. When the kinetics are slow enough, it may be better to assume that chemical speciation is fixed or frozen rather than to assume thermochemical equilibrium.

Nonideal effects are common in condensed-phase mixtures. However, in many cases, the importance of such effects may be masked by other modeling uncertainties, such as

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the vapor pressure of the pure species. Furthermore, relatively few experimental data exist from which to construct nonideal models, even for simple binary systems. Data are almost nonexistent for ternary and higher order systems. Constructing a nonideal model to treat the condensed phase or phases that would form during a severe nuclear accident would be a nearly impossible task.

4.1 Treatment of Chemical Equilibria

The approach taken in VICTORIA is to assume that mass transport is the chief bottleneck to attaining thermochemical equilibrium. Thus, under severe accident conditions, mass transport between nodes or between subregions within a node limits elemental abundances within the node or subregion; however, once species have been transported into a subregion, they rapidly attain thermochemical equilibrium. This rapid approach to equilibrium is treated in VICTORIA as being instantaneous. There are a few exceptional cases where the kinetics are modeled explicitly and these are discussed in Section 4.2.

In this chapter, and elsewhere in this report, a chemical species generally includes in its description the phase in which it is present. Thus, e.g., CsOH(g) and CsOH(c) , which represent cesium hydroxide in the gaseous and condensed phases, respectively, are considered to be two distinct chemical species.

4.1.1 Modeling Assumptions

There are two basic assumptions that are made in the VICTORIA treatment of thermochemical equilibrium. The first is that all phases are ideal. The sole exception is for control-rod alloy, as discussed in Section 4.3. Ideality is generally a good assumption for the gas phase. While it may not always be a good assumption for condensed phases, the data and justification for treating condensed phases as nonideal are lacking, as discussed earlier.

The second basic assumption is on the number of condensed phases that are treated. Originally, VICTORIA treated a single condensed phase (Heames et al., 1990). This choice, although not entirely realistic, seemed a reasonable one in view of the difficulties in evaluating the phase behavior of the complex chemical systems that would exist during a severe accident. Furthermore, some aspects of transport predictions are nearly independent of the number of phases present.

The RAFT code (Im et al., 1987) uses an approach that is diametrically opposite that used in the original VICTORIA model; the RAFT approach is to treat each condensed species as its own phase. Thus, in the RAFT approach, only pure-phase equilibrium vapor pressures need be considered in the thermochemical modeling.

The peer review committee recommended that an approach intermediate between the original VICTORIA model and the RAFT model be adopted (Mubayi et al., 1997). Their recommendation is that three distinct condensed phases be treated: an oxidic phase, a

metallic phase, and a third phase consisting of pure cesium iodide. With minor modifications, this recommendation has been incorporated into VICTORIA 2.0, as described in the following sections. This recommendation has been implemented as an option; the user can choose to treat either a single condensed phase or three condensed phases. Thus, sensitivities to this choice can be tested.

Another important assumption in the VICTORIA treatment of thermochemistry is that water (in the liquid form) is not present. If water were treated, it would be necessary to at least model aqueous chemistry and, possibly, to model transport of aqueous phases. In the past, the advantages of treating an aqueous phase did not appear to justify the complexities of such a model. However, the technology for modeling aqueous chemistry is advancing (Powers et al., 1995) and thus it may be worthwhile to reconsider this issue at a future time.

Finally, two approximations are made in the numerical treatment of thermochemical equilibrium, which is described in Part IV of this report. The first of these is that the number of moles in the condensed phase or phases changes slowly as compared with the user-prescribed time-step size. The second approximation is that the gas phase occupies most of the volume of a subregion. These two approximations are made primarily to simplify the numerical algorithms and to reduce computational costs.

4.1.2 Regions Where Equilibrium Thermochemistry Is Applied

Thermochemical equilibrium is applied in up to five subregions of a node, as illustrated in Figure 4.1. These subregions are the fuel pores, the fuel/clad gap, the control-rod layer subregion, the bulk gas subregion, and the structural layer subregion. Application of thermochemical equilibrium to each of these subregions is identical, except for the treatment of the condensed phase.

The volume of the fuel pores is the volume of the fuel times the porosity, α , as described in Chapter 2 and illustrated in Figure 2.1. By assumption, condensed-phase species deposit onto the pore surfaces and no aerosol is present in this subregion. An illustration showing an enlargement of the fuel grains (idealized as spheres), pores, and deposited film is shown in Figure 4.2.

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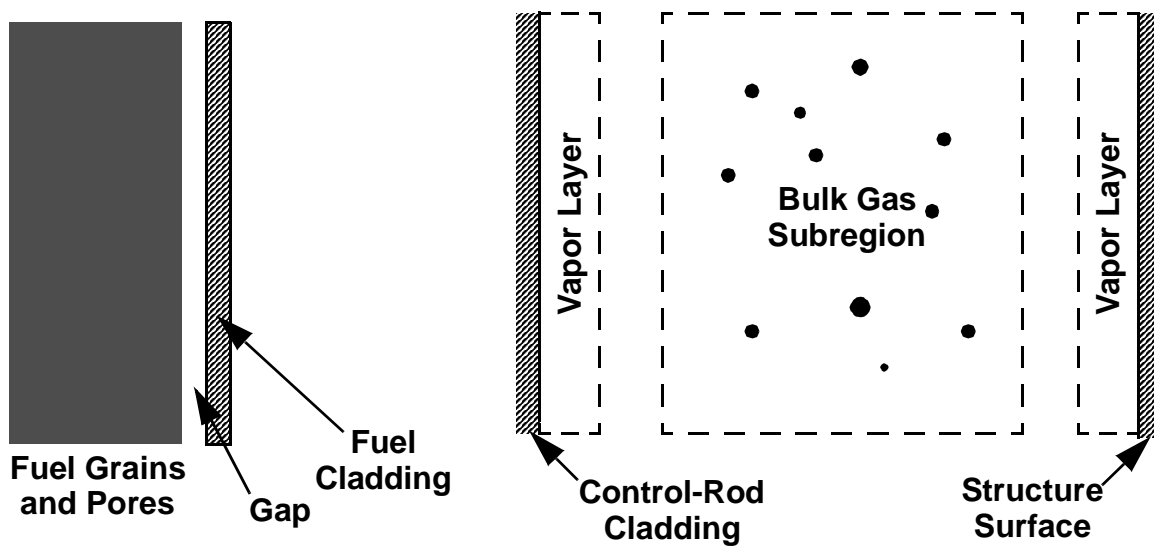


Figure 4.1. Illustration of the subregions in which thermochemical equilibrium is applied.

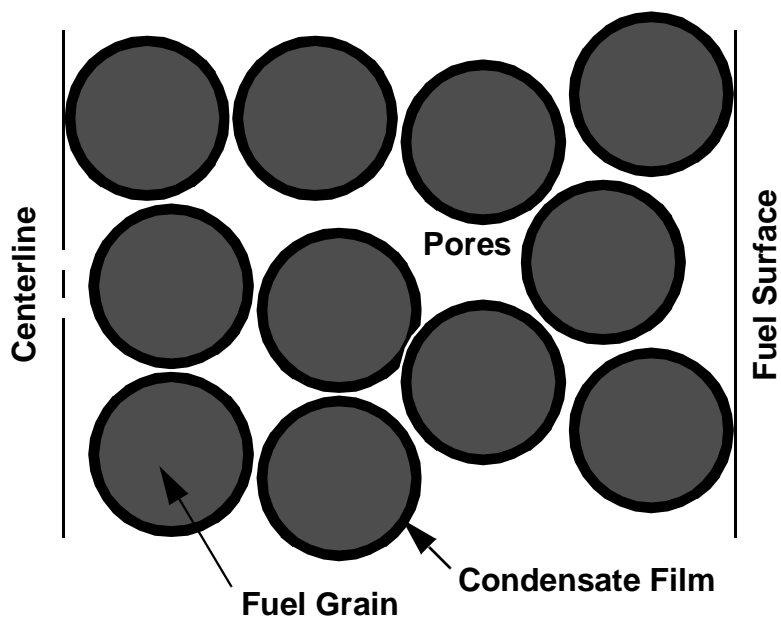


Figure 4.2. Illustration of fuel grains, pores, and deposited film representing condensate.

In the gap between the fuel and cladding, the porosity is assumed to be unity, i.e., this subregion does not collect dust or debris from the fuel pellets and is not closed by fuel pellet swelling. Thus the volume of this annular subregion is defined by its physical dimensions. Condensed-phase species are assumed to deposit onto the inner cladding surface and no aerosols are present in this subregion.

Thermochemical equilibrium is not modeled at the surface of the fuel rod. This is because modeling equilibrium there would conflict with modeling the kinetics of cladding oxidation, which is described in Subsection 4.2.1. Vapors that diffuse from the fuel rod enter the bulk gas subregion, as explained in Chapters 2 and 3.

The volume of the control-rod layer subregion is determined from the diffusion-layer thickness, as described in Chapter 3. Condensed-phase species, including control-rod alloy after failure, are assumed to be in a surface film on the control rod. Aerosol deposition onto control-rod surfaces is neglected.

The volume of the bulk gas region is determined from the volume of the node minus the volumes for the other subregions, as explained in Chapter 3. Condensation onto aerosol particles is approximated by the Fuchs-Sutugin model, which is given in Equation 3.19. No surface film for condensation of vapors exists, so the all condensed-phase species in the bulk gas subregion are in the form of aerosol particles.

The volume of the structural layer subregion is defined in the same way as the control-rod layer subregion and is also described in Chapter 3. Condensed-phase species are assumed to deposit onto a film on the structure surface. In addition, aerosols from the bulk gas subregion can deposit onto the surface film.

4.1.3 General Equilibrium Thermochemistry

Equilibrium thermochemistry is solved in a similar fashion in each subregion. The mathematical treatment begins with a statement of conservation of the number of moles of each element. This is done by summing the number of moles of an element contained in all of the species in the subregion. Since there are 26 elements in the VICTORIA database, there are 26 such balances; however, when an element does not exist in the subregion, the mass balance is trivial. Furthermore, each of the four noble-gas elements—helium, argon, krypton, and xenon—exists in only one form (i.e., as an elemental gas) so the mass balance for each of these elements is also trivial. Thus, the numerical work needed to determine thermochemical equilibrium depends on the total number of elements minus the number of noble gas elements that exist in the problem.

The second part of the mathematical treatment is to apply mass action laws (i.e., equilibrium expressions) to replace the quantity of each species in favor of the quantity of the vapor-phase elements. This reduces the number of unknowns in the system of equations to a maximum of 22, which is the number of elements in the VICTORIA database (26) minus the number of noble gas elements in the database (4). These 22 equations in 22

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unknowns are solved simultaneously, using a combination of cyclic-Newton and Newton-Raphson iterations, until a converged solution is achieved. The details of this algorithm, along with a simple example, are presented in Part IV of this report.

Previous versions of VICTORIA have assumed a single condensed phase to exist in all subregions. As described, an option has been implemented in VICTORIA 2.0 to allow three distinct condensed phases to be treated. The three phases are metallic, oxidic, and a third phase containing the iodides. The details of how species are allocated to each of the three phases are given in Part III of this report. The choice of the number of condensed phases that are treated affects thermochemical equilibrium in the following way: For the formation of a condensed-phase species, D , from three vapor-phase species, A , B , and C , the chemical equation is



where a , b , and c are the stoichiometric coefficients. The mass action law, i.e., equilibrium expression, for Equation (4.1) is

$$K = \exp\left(-\frac{\Delta G}{RT}\right) = \frac{x(D)}{p^a(A)p^b(B)p^c(C)} \quad (4.2)$$

where

- K = equilibrium coefficient ($\text{atm.}^{-(a+b+c)}$)
- ΔG = change in Gibbs free energy associated with the reaction of formation given in (4.1) ($\text{kg}\cdot\text{m}^2/\text{s}^2\cdot\text{kg}\cdot\text{mol}\cdot\text{K}$)
- R = gas constant ($\text{kg}\cdot\text{m}^2/\text{s}^2\cdot\text{kg}\cdot\text{mol}$)
- T = absolute temperature (K)
- $x(D)$ = mole fraction of condensed-phase species D in its condensed phase (dimensionless)
- $p(i)$ = partial pressure of species i (atm.)

When a single condensed phase is treated, $x(D)$ is defined as follows:

$$x(D) = \frac{C(D)}{\sum_{i \in C} C(i)} \quad (4.3)$$

where

- $C(i)$ = molar concentration of species i ($\text{kg}\cdot\text{mol}/\text{m}^3$)
- C = the set of condensed-phase species in the VICTORIA database

When three condensed phases are treated, then $x(D)$ is defined from one of the following equations, depending on whether D is a metal, an oxide, or an iodide:

$$x(D) = \frac{C(D)}{\sum_{i \in C_m} C(i)} \quad \text{if } D \in C_m \quad (4.4)$$

$$x(D) = \frac{C(D)}{\sum_{i \in C_o} C(i)} \quad \text{if } D \in C_o \quad (4.5)$$

$$x(D) = \frac{C(D)}{\sum_{i \in C_i} C(i)} \quad \text{if } D \in C_i \quad (4.6)$$

where

- C_m = the set of metallic condensed-phase species in the VICTORIA database
- C_o = the set of oxidic condensed-phase species in the VICTORIA database
- C_i = the set of iodide condensed-phase species in the VICTORIA database

Again, Part III of this report lists the condensed-phase species that are treated as metals, oxides, and iodides. In general, the metallic species are composed only of the metallic elements; the oxidic species include all those containing oxygen; and the iodides include all of the condensed-phase species containing iodine.

4.1.4 Fuel Thermochemistry

At the recommendation of the peer review committee (Mubayi et al., 1997), the treatment of fuel thermochemistry has been upgraded in VICTORIA 2.0. Earlier versions treated UO_{2+x} as being an ideal mixture of U, UO_2 , U_4O_9 , U_3O_8 , and UO_3 . The recommendation was to replace the original treatment with one based on Blackburn's model for UO_{2+x} (Blackburn, 1973). This has been done for $x > 0$, using Blackburn's original model with the Green and Leibowitz correction (Green and Leibowitz, 1981). This assumption that $x > 0$ prevents the fuel from becoming substoichiometric (i.e., prevents x from becoming negative) even under highly reducing conditions. This limitation in the current model is unimportant for nearly all situations that would arise during a severe accident because prolonged periods for which the gas phase is nearly pure hydrogen are required in order for the fuel to become substoichiometric.

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The fuel thermochemistry model is a submodel of the general thermochemistry model, with one exception. UO_{2+x} is not a species in the general thermochemistry model, but is included in the fuel thermochemistry model. In addition to UO_{2+x} , all vapor species consisting of O, H, and U in the VICTORIA database are included in this model. The list of species is thus O, O_2 , H, H_2 , HO, H_2O , U, UO, UO_2 , UO_3 , and $\text{U}(\text{OH})_2$ vapors plus UO_{2+x} in the condensed phase. The Gibbs free energies of all of the species, other than UO_{2+x} , are contained in the VICTORIA database and are listed in Part IV of this report. The Gibbs free energy for UO_{2+x} is constructed from Blackburn's expression, with the Green and Leibowitz correction, for the partial pressure of O_2 in equilibrium with UO_{2+x} :

$$\ln[p(\text{O}_2)] = 13.586 - \frac{37707}{T} + 2\ln\frac{x(2+x)}{1-x} \text{ for } 0 < x < 0.11 \quad (4.7)$$

where

$p(\text{O}_2)$ = partial pressure of O_2 (atm.)

x = excess oxygen in the fuel, as defined by UO_{2+x} (dimensionless)

The Gibbs free energy for UO_{2+x} is constructed by integrating (4.7), with the following result:

$$\begin{aligned} G(\text{UO}_{2+x}) = & G(\text{UO}_2) + \frac{x}{2}G(\text{O}_2) + 5.793RTx \\ & - 18854Rx + RTx\ln\frac{x(2+x)}{1-x} + RT\ln\frac{(2+x)^2(1-x)}{4} \end{aligned} \quad (4.8)$$

where

$G(i)$ = Gibbs free energy of species i ($\text{kg}\cdot\text{m}^2/\text{s}^2\cdot\text{kg}\cdot\text{mol}\cdot\text{K}$)

The same method is used to determine thermochemical equilibrium in the fuel as that described in the preceding subsection. Expressions for conservation of the number of moles of O, H, and U are written. Into each of these expressions is substituted the equilibrium expression for the concentration of each species in terms of the vapor-phase element concentrations. The set of three equations in three unknowns is solved simultaneously using Newton-Raphson iteration.

4.2 Treatment of Kinetic Processes

There are three special cases in the VICTORIA treatment of chemistry in which thermochemical equilibrium is not assumed. These involve oxidation of the Zircaloy cladding around the fuel, chemisorption of several species onto structural materials, and an option to "freeze" chemistry (a simple approximation to account for chemical kinetics) when

temperatures become too cold for thermochemical equilibrium to apply. Each of these models is discussed in this section.

4.2.1 Zirconium Oxidation

The current zirconium oxidation model used in VICTORIA is based on the experimental work of Urbanic and Heidrick (1978). The peer review committee recommended that this model be replaced or supplemented with one based on diffusion theory (Mubayi et al., 1997). However, because this recommendation was given a low priority by the committee, it will be considered for a future code version.

The weaknesses of the Urbanic and Heidrick model are that it assumes infinitely thick Zircaloy and that the gas phase contains an excess of steam. Nonetheless, this model is widely used because it is simple to implement and requires very little computational effort.

The relevant chemical reaction for cladding oxidation is



This reaction is treated as being irreversible. It is kinetically limited because an oxide shell builds up at the surface, which quickly restricts the rate of interaction between steam and zirconium. The kinetic expression for the rate of reaction (Urbanic and Heidrick, 1978) is

$$w^2 = k_{\text{ox}} t \quad (4.10)$$

where

w = the mass of Zr consumed per unit surface area (kg/m^2)
 k_{ox} = the kinetic coefficient of zirconium oxidation ($\text{kg}^2/\text{m}^4 \cdot \text{s}$)
 t = time (s)

Urbanic and Heidrick found the following correlations to describe the kinetic coefficient, k_{ox} , in two temperature ranges:

$$k_{\text{ox}} = 29.6 \cdot \exp(-16820/T) \text{ when } 1323 < T < 1738 \quad (4.11)$$

$$k_{\text{ox}} = 87.9 \cdot \exp(-16610/T) \text{ when } 1853 < T < 2123 \quad (4.12)$$

Between these two temperature ranges, these authors found the kinetic behavior to be discontinuous. This discontinuous behavior is ignored in the VICTORIA model for cladding oxidation. Equation (4.11) is used for temperatures up to 1763 K; Equation (4.12) is used for temperatures equal to or above 1763 K.

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The peer review committee recommended that hydrogen uptake by cladding also be modeled. However, this recommendation had a low priority and has not been implemented at this time.

4.2.2 Chemisorption

VICTORIA contains two chemisorption models that are employed by default: a model for tellurium chemisorption onto Zircaloy cladding and a model for cesium hydroxide chemisorption onto oxidized and unoxidized stainless steel surfaces. Several other optional chemisorption models can be activated by the user.

The treatment of tellurium chemisorption onto Zircaloy cladding is based on the work of Bowsher and Jenkins (1991), who performed a number of experiments using coupons made of metallic zirconium, preoxidized zirconium, Zircaloy-2, and tin. They also investigated three carrier gas compositions for a temperature range from 873 to 1273 K. They obtained the following correlation to their data:

$$v_d(\text{Te}) = 0.01 \cdot \exp \left[-\frac{4000 + 4200\sqrt{x_{\text{ox}}}}{T} + 2.0 \right] \quad (4.13)$$

where

v_d = vapor deposition velocity (m/s)
 x_{ox} = the mole fraction of zirconium in the cladding that is oxidized (dimensionless),
 $C(\text{Zr})/[C(\text{Zr}) + C(\text{ZrO}_2)]$

The rate of chemisorption is determined from the deposition velocity using the following relationship:

$$\frac{dC(i)}{dt} = -\frac{v_d A C(i)}{V} \quad (4.14)$$

where

A = surface area for chemisorption (m^2)
 V = volume of the subregion corresponding to $C(i)$ (m^3)

In this model, two tellurium species are considered: $\text{Te}(\text{g})$ and $\text{Te}_2(\text{g})$. Chemisorption onto fuel cladding is treated for both the inner and outer cladding surfaces. The temperature range for which Equation (4.13) is employed in VICTORIA is from 873 to 1673 K. This choice is based on evidence that chemisorption does not occur outside of this range (Bowsher and Jenkins, 1991).

The treatment of cesium hydroxide chemisorption onto oxidized and unoxidized stainless steel is based on the model of Vine and Clough (1991). This model describes well the results of experimental work at Sandia National Laboratories (Elrick et al., 1984) and at Winfrith Technology Centre (Bowsher et al., 1986, 1990; Dickinson, 1983; Allen et al., 1986). The model accounts for CsOH chemisorption in a water-soluble and a water-insoluble form. The important distinction in the modeling of the two forms is that chemisorption in the water-soluble form is treated as being reversible while chemisorption in the water-insoluble form is treated as being irreversible. The deposition velocities for the water-soluble and -insoluble forms, respectively, are determined from the following correlations:

$$v_{d,s}(\text{CsOH}) = 0.01 \cdot \exp\left(\frac{4330}{T} - 7.91\right) \quad (4.15)$$

$$v_{d,i}(\text{CsOH}) = 0.01 \cdot \exp\left(-\frac{7170}{T} + 2.63\right) \quad (4.16)$$

Once the deposition velocities are determined, Equation (4.14) is used to determine the molar deposition rates.

Three optional chemisorption models are available: chemisorption of tellurium onto Zircaloy (other than fuel cladding), of HI onto oxidized and unoxidized stainless steel, and of I₂ onto oxidized and unoxidized stainless steel. The procedure for switching these models on is described in Part II of this report. The vapor deposition velocity for chemisorption of tellurium (Te and Te₂) onto Zircaloy structures is identical to the one defined in Equation (4.13), which applies to fuel rod cladding. Those for the iodine species are as follows:

$$v_d(\text{HI}) = 5.5 \cdot 10^{-7} \cdot \exp\left(\frac{2.49 \cdot 10^7}{RT}\right) \quad (4.17)$$

$$v_d(\text{I}_2) = 9.0 \cdot 10^{-10} \cdot \exp\left(\frac{3.39 \cdot 10^7}{RT}\right) \quad (4.18)$$

4.2.3 “Frozen” Chemistry

A “frozen” chemistry model has been developed for VICTORIA 2.0, which accounts for chemical kinetics at low temperatures in a very simple way. Because the kinetics of reaction are unknown or poorly known for many of the reactions that would occur during a severe reactor accident, it is not practical to model chemical kinetics in a mechanistic fashion. Moreover, even if such a model could be constructed, it would be very expensive in terms of computational effort.

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The concept of the frozen chemistry model is that below a certain temperature threshold, no chemical reactions occur, only simple phase changes. Above this threshold, the standard thermochemical equilibrium treatment is used, as described in Section 4.1. In reality, the kinetics gradually become slower as temperature is decreased, the dependence on temperature being of an Arrhenius form. Furthermore, at intermediate temperatures, some chemical reactions proceed rapidly while others are very slow. The simplistic frozen chemistry model in VICTORIA does not account for any of these complications. However, it can be used to estimate the sensitivity of predictions to chemical kinetic effects. By varying the user-input threshold temperature, the model allows the user to conduct sensitivity studies in a straightforward manner.

Below the threshold temperature, the frozen chemistry model allows change of phase for all chemical forms in the database that exist as both the vapor- and condensed-phase species. The implementation of this model is simpler than the full thermochemical equilibrium model described earlier. The starting point for the frozen chemistry model is a statement of conservation of the number of moles of a chemical species, including condensed and vapor forms. Thermochemical equilibrium between ideal phases corresponds to the following relationship:

$$p(i) = p'(i)x(i) \quad (4.19)$$

where

$p'(i)$ = equilibrium vapor pressure of pure species i (atm.)

The mole fraction of species i , $x(i)$, in Equation (4.19) must be calculated for the condensed phase in which i exists. When a single condensed phase is treated, the mole fraction is defined from Equation (4.3); when three condensed phases are treated, the mole fraction is defined from Equation (4.4), (4.5), or (4.6).

Equilibrium vapor pressures are determined for the equation representing a change of phase

$$A(c) = A(g) \quad (4.20)$$

according to the following relationship

$$p'(A) = \exp(-\Delta G/RT) \quad (4.21)$$

where

ΔG = the change in Gibbs free energy for Equation (4.20) ($\text{kg}\cdot\text{m}^2/\text{s}^2\cdot\text{kg}\cdot\text{mol}\cdot\text{K}$)

The set of equations, which are coupled through the $x(i)$ s, is solved using Newton-Raphson iteration.

4.3 Treatment of Control-Rod Alloy

The total pressure inside a control rod determines whether failure of the rod results in a pressurized burst release (see Section 2.4 for a discussion of releases from control rods). The VICTORIA model for the total pressure inside a control rod is based on the work of Powers (1985). In this model, the total vapor pressure inside a control rod is calculated by summing six partial pressures.

$$P = p(\text{Ag}) + p(\text{In}) + p(\text{Cd}) + p(\text{AgIn}) + p(\text{Cd}_2) + p(\text{He}) \quad (4.22)$$

The partial pressures of the elemental vapors are calculated from the following expression

$$p(i) = x(i)\gamma(i)\exp[-\Delta G(i)/RT] \quad (4.23)$$

where

$\gamma(i)$ = activity coefficient of species i (dimensionless)

$\Delta G(i)$ = the Gibbs free energy of formation of vapor species i from the condensed-phase elements ($\text{kg}\cdot\text{m}^2/\text{s}^2\cdot\text{kg}\cdot\text{mol}\cdot\text{K}$)

For the vapor species composed of two elements, the expressions of the partial vapor pressures are slightly more complicated.

$$p(\text{AgIn}) = x(\text{Ag})x(\text{In})\gamma(\text{Ag})\gamma(\text{In})\exp[-\Delta G(\text{AgIn})/RT] \quad (4.24)$$

$$p(\text{Cd}_2) = x^2(\text{Cd})\gamma^2(\text{Cd})\exp[-\Delta G(\text{Cd}_2)/RT] \quad (4.25)$$

The activity coefficients are estimated from the Wilson equation (Powers, 1985)

$$\ln[\gamma(i)] = 1 - \ln \left[\sum_{j=1}^3 x(j)A(i,j) \right] - \sum_{k=1}^3 \left[\frac{x(k)A(k,i)}{\sum_{j=1}^3 x(j)A(k,j)} \right] \quad (4.26)$$

where

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$$A(i, j) = \frac{V(j)}{V(i)} \exp\{-[a(i, j)]/RT\} \quad \text{for } i \neq j \quad (4.27)$$

$$A(i, i) = 1 \quad (4.28)$$

Expressions for $V(i)$ and $a(i, j)$ are as follows:

$$V(\text{Ag}) = 11.343[1 + 0.000111(T - 1233)] \quad (4.29)$$

$$V(\text{In}) = 15.542[1 + 0.000118(T)] \quad (4.30)$$

$$V(\text{Cd}) = 14.015[1 + 0.000137(T - 593)] \quad (4.31)$$

$$a[\text{Ag}, \text{In}] = -3498.28 \quad (4.32)$$

$$a[\text{Ag}, \text{Cd}] = -2516.52 \quad (4.33)$$

$$a[\text{Cd}, \text{Ag}] = -1133.83 \quad (4.34)$$

$$a[\text{Cd}, \text{In}] = 6232.68 - 3.83628 \cdot 10^6/T \quad (4.35)$$

$$a[\text{In}, \text{Ag}] = 1466.00 \quad (4.36)$$

$$a[\text{In}, \text{Cd}] = -3823.49 + 3.02715 \cdot 10^6/T \quad (4.37)$$

5.0 Aerosol Processes

5.1 Background

Aerosol behavior—nucleation, growth, agglomeration, and deposition—is an important group of processes in the analysis of the consequences of a severe accident. The current understanding is that, in most cases, an aerosol is the predominant physical form of most of the fission products that would be released into the reactor containment or off-site. Even relatively volatile species like cesium iodide are generally in aerosol form by the time they reach containment. Thus, the processes relevant to aerosol formation, transport, and deposition are key to the analysis of fission product behavior during a severe accident.

The aerosol models used in VICTORIA are based on the CHARM code developed by Wheatley (1988). CHARM borrows many of its models from MAEROS (Gelbard, 1982) and TRAPMELT2 (Jordan and Kuhlman, 1985), but has been extended to treat some additional deposition mechanisms. Further, CHARM has been written to accurately evaluate agglomeration under more rapidly changing transient conditions than other, comparable aerosol codes.

VICTORIA treats aerosol behavior in the bulk gas subregion of each node, as illustrated in Figure 4.1. While aerosols can deposit onto structural surfaces, they are assumed not to deposit onto fuel or control rods. Generally, this is a good assumption because the fuel and control rod surfaces are very hot, usually hotter than the bulk gas. Models for each aspect of aerosol behavior—nucleation and growth, agglomeration, deposition, and resuspension—are described in this chapter.

5.2 Properties Affecting Aerosol Behavior

A number of gaseous and aerosol properties affect aerosol behavior. These include gas-phase density, viscosity, thermal conductivity, and heat capacity. Gas-phase viscosity is discussed in Chapter 2; density, thermal conductivity, and heat capacity are discussed in Subsection 5.2.1. Aerosol properties include the mass density and thermal conductivity of an aerosol particle. These are discussed in Subsection 5.2.2.

5.2.1 Gas Properties

The ideal gas law is used to evaluate gaseous densities. Total gas density is calculated by summing the mass concentrations of each gaseous species, as follows:

$$c(i) = \frac{p(i)M(i)}{RT} = C(i)M(i) \quad (5.1)$$

where

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$c(i)$	= mass concentration of species i (kg/m ³)
$p(i)$	= partial pressure of species i (Pa)
$M(i)$	= molecular mass of species i (kg/kg-mol)
R	= gas constant (kg·m ² /s ² ·kg-mol)
T	= absolute temperature (K)
$C(i)$	= molar concentration of species i (kg-mol/m ³)

$$\rho = \sum_{i \in G} c(i) \quad (5.2)$$

where

ρ	= gas density (kg/m ³)
G	= set of gaseous species in the VICTORIA database

Viscosities are calculated from Chapman-Enskog kinetic theory (Bird et al., 1960) for each gaseous species except steam, and from the Meyer correlation (Meyer et al., 1967) for steam. The Wilke semiempirical formula (Bird et al. 1960) is used to determine the viscosity of a mixture. These relationships are given in Equations (2.26) through (2.29).

Thermal conductivities of all gaseous species but steam are calculated from Eucken's semiempirical equation (Bird et al., 1960), which is valid for polyatomic gases.

$$k(i) = \left[C_p(i) + \frac{5R}{4M(i)} \right] \mu(i) \quad (5.3)$$

where

$k(i)$	= thermal conductivity of gaseous species i (W/m·K)
$C_p(i)$	= heat capacity of gaseous species i (W/kg·K)
$\mu(i)$	= viscosity of pure species i (kg/m·s)

The thermal conductivity of steam is calculated from the MATPRO correlation (Hohorst, 1990), which is the following:

$$k(\text{H}_2\text{O}) = 1.76 \cdot 10^{-2} + 5.87 \cdot 10^{-5} \cdot X + 1.04 \cdot 10^{-7} \cdot X^2 - 4.51 \cdot 10^{-11} \cdot X^3 \text{ for } X < 973 \quad (5.4)$$

$$k(\text{H}_2\text{O}) = 1.28 \cdot 10^{-3} + 4.44 \cdot 10^{-6} \cdot X^{1.45} \text{ for } X \geq 973 \quad (5.5)$$

where

X	= temperature (°C), $T - 273.16$
-----	----------------------------------

Gaseous heat capacities are determined from classical theory (Lee et al., 1963):

$$C_p(i) = \frac{N(i) + 3}{2} \frac{R}{M(i)} \quad (5.6)$$

where

$N(i)$ = the number of atoms in a molecule of species i (dimensionless)

The thermal conductivity of a gaseous mixture is estimated by a method analogous to the Wilke semiempirical expression used for viscosity in Equation (2.28) (Bird et al., 1960).

$$k_g = \sum_{i \in G} \frac{x(i)k(i)}{\sum_{j \in G} x(j)\Phi_{ij}} \quad (5.7)$$

where

k_g = thermal conductivity of gas (W/m·K)

Φ_{ij} = a dimensionless parameter defined in Equation (2.29) (dimensionless)

5.2.2 Aerosol Properties

Aerosol particles are characterized by mass in the VICTORIA code. Since many of the correlations for aerosol behavior depend on particle radius, a determination of particle density is essential. VICTORIA contains a database for the density of each pure species, $\rho(i)$, which is given in Part III of this report. Densities of mixtures of species are calculated by mass averaging according to the following equation:

$$\rho_a = \frac{\sum_{i \in C} c(i)\rho(i)}{\sum_{i \in C} c(i)} \quad (5.8)$$

where

ρ_a = density of an aerosol particle (kg/m³)

$c(i)$ = mass of aerosol species i per volume of bulk gas (kg/m³)

$\rho(i)$ = density of pure condensed-phase species i (kg/m³)

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C = set of condensed-phase species in the VICTORIA database

Thermal conductivities of aerosol particles are important for estimating thermophoretic deposition. Thermal conductivities are estimated by volume weighting, regardless of whether one or three phases are treated:

$$k_a = \frac{20 \cdot \sum_{i \in C_m} c(i)/\rho(i) + 0.6 \cdot \left[\sum_{i \in C_o} c(i)/\rho(i) + \sum_{i \in C_i} c(i)/\rho(i) \right]}{\sum_{i \in C} c(i)/\rho(i)} \quad (5.9)$$

where

k_a = thermal conductivity of an aerosol particle (W/m·K)

In this approximation for thermal conductivity, the metallic phase is taken to have a thermal conductivity of 20 W/m·K; nonmetallic phases are taken to have a thermal conductivity of 0.6 W/m·K. Thermal conductivity is calculated in the same manner whether the mixture is at a molecular or mechanical level.

5.2.3 Dimensionless Numbers

Several dimensionless numbers are important for modeling aerosol behavior. The first of these is the particle Knudsen number, the ratio of the mean free path to the particle radius, which is expressed as

$$Kn = l_p / r_a \quad (5.10)$$

where

Kn = particle Knudsen number (dimensionless)
 l_p = mean free path of a gas molecule (m), as defined in Equation (3.20)
 r_a = radius of aerosol particle (m)

The particle Knudsen number is a measure of the relative importance of molecular dynamic effects and continuum effects. Thus, for small values of Knudsen number, continuum theory applies; for large values of the Knudsen number, molecular theory applies. Theoretical estimations are most difficult at intermediate values of the Knudsen number, where neither molecular nor continuum theories apply. Many models use an empirical representation to bridge between continuum and molecular theoretical results.

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The particle Schmidt number, the ratio of viscous drag force to Brownian force, is defined as

$$Sc = \frac{\mu}{\rho k_B T B} \quad (5.11)$$

where

- μ = gas-phase dynamic viscosity (kg/m·s), as defined in Equation (2.28)
- ρ = gas-phase density (kg/m³), as defined in Equation (5.2)
- k_B = Boltzmann's constant (kg·m²/s²·K·molecule)
- B = particle mobility (s/kg), as defined by the following equations:

$$B = B_{St} \cdot Cn \quad (5.12)$$

$$B_{St} = \frac{1}{6\pi\chi_d\mu r_a} \quad (5.13)$$

$$Cn = 1 + k_1 Kn + k_2 Kn \exp(-k_3/Kn) \quad (5.14)$$

where

- B_{St} = coefficient in Stokes mobility law (s/kg)
- Cn = Cunningham's slip correction factor (Cunningham, 1910) (dimensionless)
- χ_d = dynamic shape factor, an empirical, dimensionless correction factor for nonspherical particles (unity for spherical particles) (dimensionless) [1]
- k_1, k_2, k_3 = empirical, dimensionless constants (dimensionless)

Default values for k_1 , k_2 , and k_3 are 1.25, 0.41, and 0.88, respectively, and are from Davies (1966).

The particle Stokes number is defined as

$$St = \frac{4Cn\rho_a r_a^2 U}{9\mu D_H} \quad (5.15)$$

where

- U = gas speed (m/s), $\sqrt{u^2 + v^2}$
- u = radial component of velocity (m/s)
- v = axial component of velocity (m/s)
- D_H = hydraulic diameter (m)

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Other dimensionless quantities that are used to predict aerosol behavior, which include Re and Nu, are defined as follows:

- Re = Reynolds number (dimensionless), $(\rho U D_H)/\mu$
Nu = Nusselt number (dimensionless), $(h D_H)/k$
 h = heat transfer coefficient ($\text{W}/\text{m}^2 \cdot \text{K}$)

Correlations used for Nu are given in Equations (3.1) through (3.5).

5.3 Governing Equation

Aerosol behavior is governed by the following integral equation:

$$\frac{\partial}{\partial t} N(m) = \frac{1}{2} \int_0^m \Phi(\omega, m - \omega) N(\omega) N(m - \omega) d\omega - N(m) \int_0^\infty \Phi(\omega, m) N(\omega) d\omega - R(m) + S(m) \quad (5.16)$$

where

- $N(m)$ = aerosol number concentration of particles of mass m ($1/\text{m}^3$)
 $\Phi(\omega, m)$ = agglomeration kernel ($\text{m}^3/\text{kg} \cdot \text{t}$), i.e., a measure of the rate at which particles of mass ω agglomerate with particles of mass m
 m, ω = mass of an aerosol particle (kg)
 $R(m)$ = volumetric removal rate of particles of size m due to deposition ($1/\text{m}^3 \cdot \text{s}$)
 $S(m)$ = volumetric source rate of particles of size m ($1/\text{m}^3 \cdot \text{s}$)

The terms in Equation (5.16), from left to right, represent the following quantities: (1) the rate of increase of the number of particles of mass m per volume of gas; (2) the agglomeration by collision of particles of mass ω and $m - \omega$ to form new particles of mass m ; (3) the loss of particles of mass m by agglomeration with other particles of mass ω to form a new particle of mass $m + \omega$; (4) removal of particles of mass m by deposition; and (5) the source rate of particles of mass m , including resuspension of previously deposited aerosols. All terms in Equation (5.16) are on a volumetric basis.

Nucleation and growth, agglomeration, deposition, and resuspension of aerosol particles are discussed in the following sections. The numerical solution of Equation (5.16) is discussed in Part IV of this report.

5.4 Nucleation and Growth

Nucleation and growth of aerosol particles are not described by Equation (5.16); rather, these processes are treated independently. Condensation of vapors is determined according to thermochemical equilibrium, as described in Chapter 4. Because the condensed phase in the bulk gas region is in the form of aerosols, by assumption, condensation is a source for nucleation and growth of aerosol particles. Likewise, evaporation results in a declivity of aerosol particles. While the discussion is couched in terms of condensation and growth of aerosol particles in this section, the arguments apply equally well to the evaporation and declivity of those particles.

VICTORIA contains a simple heterogeneous nucleation model. When no aerosols are present, the condensing mass is placed in the smallest aerosol mass bin (i.e., size class) defined by the input parameters. This model is a simple way to account for aerosol seeds, which must be ubiquitous during a severe accident. While it might seem that the predicted aerosol size distribution could be sensitive to the choice of the smallest aerosol mass bin defined in a calculation, this has proven not to be the case. Sensitivity studies have demonstrated that memory of the initial size of the nucleating particles is quickly erased by agglomeration. However, when aerosol number concentrations are extremely small, the initial size of nucleating particles could have an influence on the final size distribution. In such cases, it would be prudent for the user to investigate the sensitivity of predicted results to the choice of the smallest aerosol mass bin.

The choice to omit a homogeneous nucleation model in VICTORIA is based on several factors:

1. It is unlikely that homogeneous nucleation is important during severe accidents because of the buildup of oxides and deposits during normal operation. These deposits should provide a large source of aerosol seed particles that would dominate the competition for aerosol nucleation under severe accident conditions.
2. Homogeneous nucleation is a difficult problem to solve numerically, generally requiring very small time steps. In numerical terminology, the equations are very stiff.
3. Homogeneous nucleation usually occurs in a very narrow front. In order to resolve this front, a fine nodalization is often required. Furthermore, the location of the front may not be stationary; thus, a whole region may need to be finely nodalized.

For these reasons, the developers of VICTORIA chose not to model homogeneous nucleation. Results from the Falcon International Standard Problem (Williams, 1994) indicated that modeling of homogeneous nucleation does not provide an advantage over the simpler modeling approach used in VICTORIA unless thermal profiles are known at a highly detailed level.

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Once aerosol particles form, whether by homogeneous or heterogeneous nucleation, they continue to grow as condensation of vapors progresses. This usually occurs when vapors and aerosols are transported into cooler and cooler regions of the reactor coolant system. Condensation of vapors onto aerosols is modeled using the Fuchs-Sutugin growth law (Hidy and Brock, 1971), as described in Section 3.4.

5.5 Agglomeration

Mechanisms that result in collision and subsequent coalescence of aerosol particles are classified as agglomeration processes. Four such processes are treated by VICTORIA. These are agglomeration by Brownian motion, gravitational settling, turbulent shear, and turbulent inertial mechanisms. Each of these processes induces relative velocities between aerosol particles and therefore can cause collisions. Expressions for the agglomeration rates by these four mechanisms define the agglomeration kernel used in Equation (5.16), as described below.

Collisions between particles do not necessarily result in coalescence or agglomeration. The probability that two particles will coalesce when they collide is called the particle-to-particle sticking efficiency. While the default sticking efficiency in VICTORIA is unity, this parameter can be modified in the input. Likewise, a collision shape factor accounts for variations in the probability for a collision between two particles when their shapes are not spherical. This parameter has a default value of unity, which represents spherical particles, but may be modified in the input.

5.5.1 Brownian Agglomeration

The Brownian agglomeration rate is estimated according to the following equation:

$$\Phi_B(m, \omega) = 4\pi\kappa_B T [B(m) + B(\omega)] \chi_c [r_a(m) + r_a(\omega)] Fu(m, \omega) \quad (5.17)$$

where

- $\Phi_B(m, \omega)$ = agglomeration rate of particles of mass m with particles of mass ω due to Brownian diffusion ($\text{m}^3/\text{kg}\cdot\text{t}$)
- $B(m)$ = mobility of particle with mass m , as defined by Equations (5.12) through (5.14) (s/kg)
- χ_c = collisional shape factor (dimensionless) [1]
- $r_a(m), r_a(\omega)$ = radii of particles with mass m and ω , respectively (m)
- $Fu(m, \omega)$ = Fuchs factor (Fuchs, 1989) as defined by the following equations (m^2)

$$\frac{1}{Fu(m, \omega)} = \frac{1}{Fu_1(m, \omega)} + \frac{1}{Fu_2(m, \omega)} \quad (5.18)$$

$$Fu_1(m, \omega) = \varepsilon_s \frac{r_a(m) + r_a(\omega)}{\kappa_B T [B(m) + B(\omega)]} \sqrt{\frac{8\kappa_B T}{\pi} \left(\frac{1}{m} + \frac{1}{\omega} \right)} \quad (5.19)$$

$$Fu_2(m, \omega) = 1 + \frac{2\sqrt{(\tilde{a}_m^2 + \tilde{a}_\omega^2)}}{r_a(m) + r_a(\omega)} \quad (5.20)$$

$$\tilde{a}_m = \frac{[r_a(m) + a_m]^3 - [r_a^2(m) + a_m^2]^{3/2}}{3r_a(m)a_m} - r_a(m) \quad (5.21)$$

$$a_m = B(m) \sqrt{\frac{2\kappa_B T m}{\pi}} \quad (5.22)$$

where

- $Fu_1(m, \omega)$ = factor from kinetic theory, i.e., when particle size is less than the mean free path of a gas molecule (m^2)
- $Fu_2(m, \omega)$ = factor from diffusion theory (Sitarski and Seinfeld, 1977), i.e., when particle size is greater than the mean free path of a gas molecule (m^2)
- ε_s = particle-to-particle sticking efficiency (dimensionless)

5.5.2 Gravitational Agglomeration

The gravitational agglomeration rate is estimated according to the following equation:

$$\Phi_G(m, \omega) = \varepsilon_s \varepsilon_{PK}(m, \omega) \chi_c^2 [r_a(m) + r_a(\omega)]^2 |v_g(m) - v_g(\omega)| \quad (5.23)$$

where

- $\Phi_G(m, \omega)$ = agglomeration rate of particles of mass m with particles of mass ω due to gravitational settling ($m^3/\text{kg}\cdot\text{t}$)
- ε_{PK} = collision efficiency correction factor due to Prupacher and Klett (dimensionless)
- $v_g(m), v_g(\omega)$ = gravitational settling velocity of a particle of mass m and ω , respectively (m/s)

For the Prupacher and Klett collision efficiency, VICTORIA uses the recommendation of Dunbar et al. (1984):

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$$\varepsilon_{PK}(m, \omega) = \frac{1}{2} \frac{\min^2[r_a(m), r_a(\omega)]}{[r_a(m) + r_a(\omega)]^2} \quad (5.24)$$

where the function min indicates a minimum value. Particle settling velocities are evaluated from the following expression:

$$v_g(m) = g \cdot m \cdot B(m) \quad (5.25)$$

A correction to account for the density of the gas phase is not included because this correction is negligible even at high system pressures.

5.5.3 Turbulent Shear Agglomeration

Turbulent shear can cause particles that follow flow pathlines to collide with one another. This occurs because particles on different streamlines are traveling at different speeds. Turbulent shear agglomeration is a result of this effect.

The turbulent shear agglomeration rate is estimated from the following expression, which is due to Saffman and Turner (1956):

$$\Phi_S(m, \omega) = \varepsilon_s \varepsilon_{PK}(m, \omega) \chi_c^3 [r_a(m) + r_a(\omega)]^3 \sqrt{\frac{8\rho\pi\phi_T}{15\mu}} \quad (5.26)$$

where

$\Phi_S(m, \omega)$ = agglomeration rate of particles of mass m with particles of mass ω due to turbulent shear ($\text{m}^3/\text{kg}\cdot\text{s}$)

ϕ_T = turbulent energy dissipation rate per unit mass (m^2/s^3)

Deliachasios and Probstein (1974) offer the following equation for the turbulent energy dissipation rate:

$$\phi_T = \frac{0.03146U^3}{D_H \text{Re}^{3/8}} \quad (5.27)$$

5.5.4 Turbulent Inertial Agglomeration

Turbulent inertial agglomeration results when particle trajectories depart from flow pathlines. This departure is caused by the mass of an aerosol particle, which causes it to accelerate or decelerate more slowly than a gas particle (molecule). Because of the chaotic motions of a highly turbulent flow, turbulent inertial agglomeration can dominate over other agglomeration mechanisms.

The turbulent inertial agglomeration rate is also estimated from Saffman and Turner (1956) according to the following expression:

$$\Phi_I(m, \omega) = \varepsilon_s \varepsilon_{PK}(m, \omega) \chi_c^2 [r_a(m) + r_a(\omega)]^2 \left(\frac{512 \rho \pi^3 \phi_T^3}{15 \mu} \right)^{1/4} \frac{|v_g(m) - v_g(\omega)|}{g} \quad (5.28)$$

where

$\Phi_I(m, \omega)$ = agglomeration rate of particles of mass m with particles of mass ω due to turbulent inertia ($\text{m}^3/\text{kg}\cdot\text{t}$)

5.5.5 Summation of Agglomeration Terms

According to Saffman and Turner (1956), the two turbulent agglomeration terms, $\Phi_S(m, \omega)$ and $\Phi_I(m, \omega)$, should be added in a root mean fashion. Using this recommendation, the agglomeration kernel is defined as follows:

$$\Phi(m, \omega) = \Phi_B(m, \omega) + \Phi_G(m, \omega) + \sqrt{\Phi_S^2(m, \omega) + \Phi_I^2(m, \omega)} \quad (5.29)$$

Dunbar et al. (1984) point out that the reasoning used by Saffman and Turner also applies to the gravitational contribution to the agglomeration kernel, $\Phi_G(m, \omega)$. Thus they argue that the last three terms in Equation (5.29) should be summed in a root mean square sense. While the correct summation rule for the contributions to the agglomeration kernel remains a matter of some disagreement, the VICTORIA treatment of agglomeration follows the Saffman and Turner recommendation.

5.6 Deposition

VICTORIA accounts for five aerosol deposition mechanisms: (1) gravitational settling, (2) turbulent deposition, (3) diffusive deposition under laminar conditions (i.e., from Brownian motion), (4) thermophoretic deposition, and (5) inertial deposition due to flow irregularities. The deposition velocities for each of these mechanisms are described in the following subsections.

5.6.1 Gravitational Settling

The settling velocity for an aerosol particle, v_g , is given in Equation (5.25). This settling velocity is the deposition velocity for gravitational settling, i.e.,

$$u_g = v_g \quad (5.30)$$

where

u_g = deposition velocity due to gravitational settling (m/s)

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5.6.2 Turbulent Deposition

Two separate correlations are used to estimate turbulent deposition: the first is for submicron particles ($r_a < 10^{-6}$ m) and the second is for supermicron particles ($r_a > 10^{-6}$ m). The model for the deposition of submicron particles is due to the theoretical model of Davies (1966), which is

$$u_{t,s} = \frac{Sc^{-2/3} \tilde{v}}{14.5 \left\{ \frac{1}{6} \ln \left[\frac{(1 + \phi)^2}{1 - \phi + \phi^2} \right] + \frac{1}{\sqrt{3}} \operatorname{atan} \left[\frac{2\phi - 1}{\sqrt{3}} \right] + \frac{\pi}{\sqrt{3}} \right\}} \quad (5.31)$$

where

$u_{t,s}$ = turbulent deposition velocity for submicron particles (m/s)
 \tilde{v} = friction velocity (m/s), as defined by the following expression:

$$\tilde{v} = U \sqrt{\frac{f}{2}} \quad (5.32)$$

f = Fanning friction factor (dimensionless)
 ϕ = $Sc^{1/3}/2.9$

The Fanning friction factor is calculated from the following correlation, which is valid for turbulent flow through aerodynamically smooth pipes (Colebrook, 1939):

$$\frac{1}{2\sqrt{f}} = 1.74 - 2 \log \left[\frac{18.7}{2Re\sqrt{f}} \right] \quad (5.33)$$

For the contribution from supermicron particle deposition in a turbulent flow field, the following correlation derived by Sehmel (1970) is used:

$$u_{t,s} = 1.47 \cdot 10^{-16} \left(\frac{\rho_a}{1000} \right)^{1.01} \left(\frac{2 \cdot 10^4 r_a}{D_H} \right)^{2.1} Re^{3.02} \tilde{v} \quad (5.34)$$

where

$u_{t,s}$ = turbulent deposition velocity for supermicron particles (m/s)

Either Equation (5.31) or (5.34) defines the turbulent deposition velocity, u_t , depending on whether the particle size is less than or greater than 1μ .

5.6.3 Diffusive Deposition

The particle deposition velocity from diffusion in a laminar flow is estimated by the following expression:

$$u_d = (\psi - 1) \frac{D_H}{L} U \quad (5.35)$$

where

ψ = empirical coefficient, which is correlated to the data of Gormley and Kennedy (1949) as follows:

$$\psi = 1 - 4.07H^{2/3} + 2.4H + 0.446H^{4/3} \text{ when } H \leq 0.0156 \quad (5.36)$$

$$\psi = 0.819 \exp(-7.314H) + 0.0975 \exp(-44.6H) + 0.0325 \exp(-114H) \text{ when } H > 0.0156 \quad (5.37)$$

where

H = measure of diffusive-to-convective transport (dimensionless),
 $(2LD_B)/(D_H^2 U)$
 L = length over which deposition takes place (m)
 D_B = Brownian diffusivity (m²/s)
 $= k_B TB$

5.6.4 Thermophoretic Deposition

Thermophoretic deposition is the motion of aerosol particles due to a thermal gradient. Thermophoretic forces arise from collisions between aerosol particles and fluid molecules. Since the mean momentum transfer due to these collisions is proportional to the square of the gas temperature, a net force is exerted on the aerosol in the direction of the lower temperature region.

A hydrodynamic analysis of this phenomenon was performed by Brock (1962). The formula he derived is still regarded as the most reliable and is used in most aerosol physics codes. The Brock formula for thermophoretic deposition is

$$u_T = \frac{-2C_s \left(\frac{k_g}{k_a} + C_t \text{Kn} \right) \frac{\mu \text{Cn}}{\rho} \frac{T_g - T_s}{T_g \delta_T}}{(1 + 3C_m \text{Kn}) \left(1 + 2 \frac{k_g}{k_a} + 2C_t \text{Kn} \right)} \quad (5.38)$$

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where

u_T	=	deposition velocity for thermophoresis (m/s)
C_s	=	thermal slip coefficient (dimensionless) [1.17]
C_t	=	thermal accommodation coefficient (dimensionless) [2.18]
C_m	=	momentum accommodation coefficient (dimensionless) [1.14]
T_g	=	temperature of gas (K)
T_S	=	temperature of structure (K)
δ_T	=	thermal boundary layer thickness (m), as defined in Equations (3.6) and (3.7)

The default values used in VICTORIA for the thermal slip, thermal accommodation, and momentum accommodation coefficients given here are those recommended by Talbot et al. (1980); they demonstrate good agreement with experimental data across a broad range of Knudsen numbers.

5.6.5 Inertial Deposition from Flow Irregularities

Five models for aerosol deposition due to geometrically induced flow irregularities are available in VICTORIA: (1) deposition in 90° pipe bends; (2) deposition in abrupt contractions in pipes; (3) deposition in upcomer cyclone-type steam separators; (4) deposition in chevron-type steam dryers; and (5) deposition near the mouth of a vena contracta. These deposition models are discussed in this subsection.

Deposition induced by flow irregularities is generally by impaction of aerosol particles against surfaces in the vicinity of the geometrical irregularity. Deposition is caused by inertial effects; aerosol particles are unable to follow flow streamlines because the aerosol is more dense than the surrounding fluid. Some of the aerosol particles thus collide with a surface and deposit. Generally, larger aerosol particles deposit preferentially over smaller ones, which are able to follow fluid streamlines more closely.

Pipe Bends

The model used in VICTORIA for deposition in 90° pipe bends under turbulent conditions (i.e., $Re \geq 2300$) is based on the experimental and theoretical work of Pui et al. (1987). Their experiments covered a range of Reynolds numbers from 10^2 to 10^4 . They found that an exponential relationship between Stokes number and deposition efficiency correlated well with their data. This relationship is

$$\eta_b = 1 - 10^{-0.963St} \quad (5.39)$$

where

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η_b = deposition efficiency due to flow irregularity (dimensionless)

The particle Stokes number is defined in Equation (5.15). Deposition efficiency is the fraction of aerosol particles of a specific size that deposit. More specifically for Equation (5.39), the deposition efficiency represents the fraction of aerosol particles that deposit near the pipe bend because of inertial effects induced by curvature of the fluid streamlines. Deposition efficiency is converted to deposition velocity in VICTORIA by the following definition:

$$u_b = \eta_b \frac{U V_B}{L A} \quad (5.40)$$

where

u_b = deposition velocity for flow through a bend (m/s)

V_B = volume of bulk gas subregion (m³), as defined in Chapter 3

A = surface area for aerosol deposition (m²)

To a first order of approximation, deposition in a pipe bend is independent of the radius of curvature of the bend; however, according to Pui et al., Equation (5.39) is valid for bends of small to intermediate radii of curvature. While this is not very precise terminology, the equation should be applicable to bends with a radii of curvature on the order of several pipe radii. This equation could overpredict deposition in a bend where the radius of curvature is an order of magnitude or more greater than the pipe radius.

Deposition in 90° bends under laminar flow conditions (i.e., $Re < 2300$) is based on the data of Cheng and Wang (1975, 1981), which was measured for a Reynolds number of 10^3 . The following correlations are used to fit these data:

$$\eta_b = 0 \text{ when } St \leq 0.117 \quad (5.41)$$

$$\eta_b = 1 \text{ when } St \geq 1.5 \quad (5.42)$$

and between these limits, VICTORIA interpolates linearly using the following data table:

Table 5.1: Deposition Efficiency in Laminar Flow for a 90° Pipe Bend

St	0.117	0.200	0.242	0.300	0.315	0.350	0.377	0.400	0.425	0.500	0.600	0.700	0.800	0.900	1.000	1.100	1.200	1.500
η_b	0.000	0.118	0.200	0.340	0.400	0.500	0.600	0.657	0.700	0.792	0.862	0.896	0.920	0.940	0.960	0.974	0.990	1.000

Aerosol Processes

Abrupt Contraction

Abrupt contractions exist in many of the small-scale experiments that have been analyzed with VICTORIA. A sudden contraction can also be used to represent flow into a steam generator tube. The model for deposition in an abrupt pipe contraction (illustrated in Figure 5.1) is taken from the work of Ye and Pui (1990). Their correlation is based on numerical calculations for laminar flow using a fluid-flow code (Patankar, 1980) to predict particle trajectories in the vicinity of the sudden contraction, and was found to agree well with experimental data. Ye and Pui's correlation is in the form of the dependence of deposition efficiency on tube diameters upstream and downstream of the contraction and on the particle Stokes number, which is given in the following equations:

$$\eta_b = 0 \text{ for } X < 0.213 \quad (5.43)$$

$$\eta_b = \left[1 - \left(\frac{D_o}{D_i} \right)^2 \right] [1 - \exp(1.721 - 8.557X + 2.227X^2)] \text{ for } 0.213 \leq X \leq 1.95 \quad (5.44)$$

$$\eta_b = 1 - \left(\frac{D_o}{D_i} \right)^2 \text{ for } 1.95 < X \quad (5.45)$$

$$X = \sqrt{\text{St}} \left(\frac{D_o}{D_i} \right)^{0.31} \quad (5.46)$$

where

D_o = pipe diameter at the outlet of the sudden contraction (m)

D_i = pipe diameter at the inlet of the sudden contraction (m)

St = particle Stokes number, based on the inlet velocity and the outlet diameter (dimensionless), $\frac{4Cn\rho_a r_a^2 U_i}{9\mu D_o}$

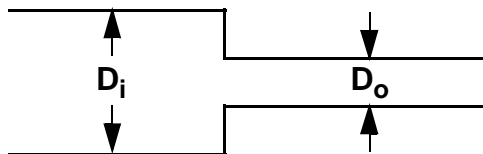


Figure 5.1. Illustration of a sudden contraction.

While the Ye and Pui correlation is constructed for laminar flow conditions, it is believed to apply to turbulent conditions as well, although to the authors' knowledge, this has not

been established. This model treats sudden contractions where the upstream diameter, D_i , is up to ten times the downstream diameter, D_o . The equation below for a vena contracta is useful when the ratio of upstream to downstream diameter is greater than 10.

Steam Separators

VICTORIA's models for steam separators and dryers are taken from the RAFT code (Im et al., 1987). These models are developed for boiling water reactors. Although they may be applicable for pressurized water reactors, it turns out that the flow rates through the secondary side of a steam generator in a PWR are too slow for these deposition mechanisms to be active during sequences such as a steam generator tube rupture, even with multiple tube ruptures. Thus, these models are useful primarily for studies of BWR accident sequences.

The first of the two BWR models is for aerosol deposition in an upcomer cyclone-type steam separator, as illustrated in Figure 5.2. A centrifugal force for inertial collection of particles is imparted by a guide vane, which invokes a swirling flow. Im et al. express the deposition efficiency as

$$\eta_b = 1 - \left(\frac{R_d}{R_v}\right)^2 \quad (5.47)$$

where

- R_d = the radial coordinate of a particle that will just deposit on the vortex tube wall at the top of the vortex tube (m)
- R_v = the radius of the vortex tube (m)

The value of R_d/R_v can be determined from the values of a function, which is defined as follows:

$$f\left(\frac{R_d}{R_v}\right) = 1.29228 \text{St} \left(\frac{H_v}{R_v}\right) (\cot \theta)^2 \quad (5.48)$$

where

- H_v = height of a vortex tube (m)
- θ = vane angle (radians)
- St = particle Stokes number, $\frac{4C_n \rho_a r_a^2 U}{18\mu R_v}$

Aerosol Processes

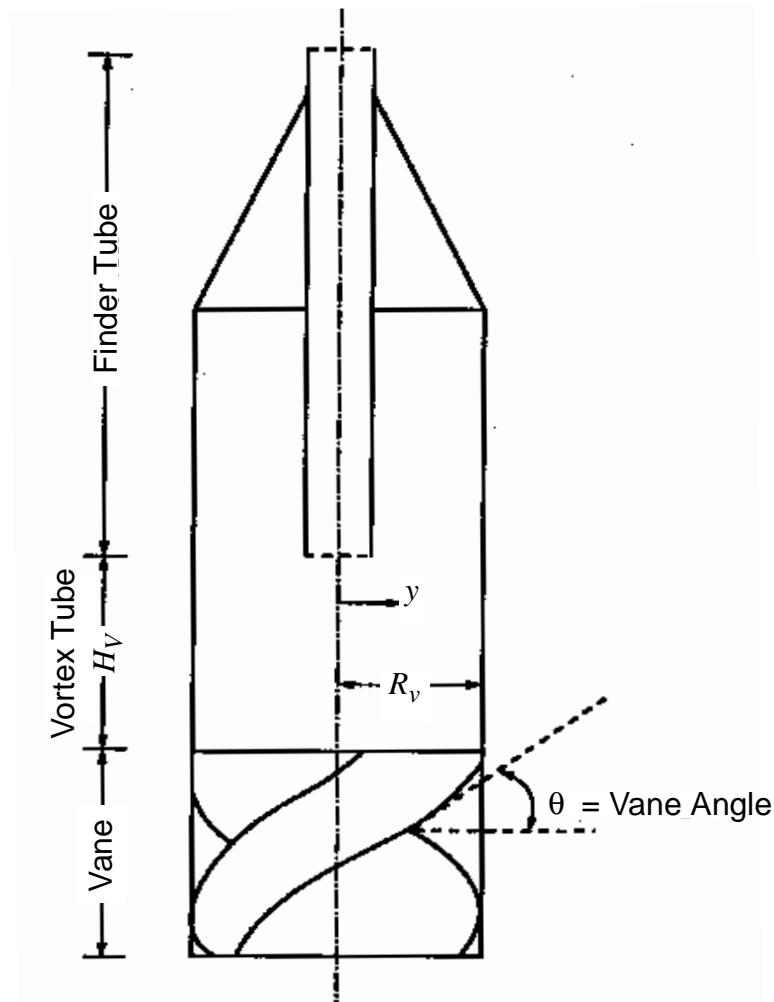


Figure 5.2. Illustration of an upcomer cyclone-type steam separator.

The variable $f(R_d/R_v)$ is determined from Equation (5.48) for a particular Stokes number (which depends on aerosol particle size). Then (R_d/R_v) is determined by linear interpolation from the following lookup table:

Table 5.2: Data for Deposition Efficiency in an Upcomer Cyclone-Type Steam Separator

R_d/R_v	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	0.50
$f(R_d/R_v)$	0.70218	0.69925	0.69205	0.68194	0.66958	0.65529	0.63923	0.62140	0.60176	0.58014	0.55634
R_d/R_v	0.55	0.60	0.65	0.70	0.75	0.80	0.85	0.90	0.95	1.00	
$f(R_d/R_v)$	0.53002	0.50077	0.46800	0.43095	0.38853	0.33921	0.28073	0.20955	0.11972	0.00000	

With (R_d/R_v) determined, deposition efficiency is calculated from Equation (5.48) and converted to deposition velocity using Equation (5.40).

Steam Dryers

The RAFT model for aerosol deposition in steam dryers (illustrated in Figure 5.3) is expressed as follows:

$$\eta_b = 1 - [0.24(5.17 - \cos \Theta) - 2.3(1 - \cos \Theta)St]^N \quad (5.49)$$

where

- Θ = turning angle of a chevron guide
- St = particle Stokes number, $\frac{4C_n \rho_a r_a^2 U}{9\mu D_v}$
- N = number of bends in a steam dryer
- D_v = perpendicular spacing between vanes (m)

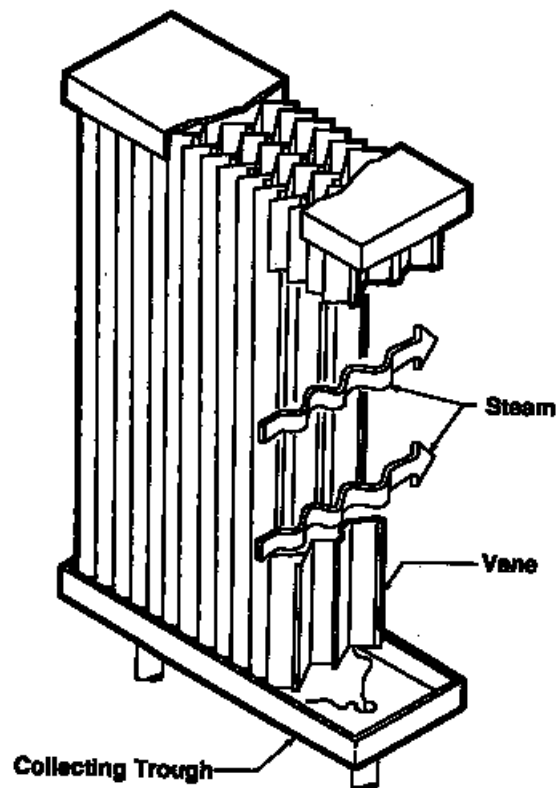


Figure 5.3. Illustration of a chevron-type steam dryer.

Aerosol Processes

Vena Contracta

The flow from the upper plenum of a reactor vessel into a hot leg is reasonably represented as a vena contracta. The model used in VICTORIA for deposition near a vena contracta (illustrated in Figure 5.4) is based on the work of Belyaev and Levin (1972). Their expression for deposition efficiency is the following:

$$\eta_b = \left[1 - \left(\frac{D_o}{D_i} \right)^2 \right] \left\{ 1 - \left[1 + 2St + 0.617 \left(\frac{D_o}{D_i} \right)^2 St \right]^{-1} \right\} \quad (5.50)$$

Equation (5.50) is valid when $0.18 < St < 2.03$ and $0.17 < (D_o/D_i)^2$, although it is well behaved outside of these limits. The inlet diameter, D_i , in Equation (5.50) does not necessarily indicate an actual tube diameter; it can also indicate the effective upstream diameter of the stream tube that enters the pipe for which deposition is being modeled.

5.6.6 Summation of Deposition Velocities

Deposition is calculated separately for three orientations of structural surfaces: ceilings, walls, and floors. The primary difference between them is the gravitational settling term; however, deposition due to flow irregularities is ascribed to walls. Deposition velocities are linearly summed as follows:

$$u_c = u_d + u_t + u_{T,c} - u_g \quad (5.51)$$

$$u_w = u_d + u_t + u_{T,w} + u_b \quad (5.52)$$

$$u_f = u_d + u_t + u_{T,f} + u_g \quad (5.53)$$

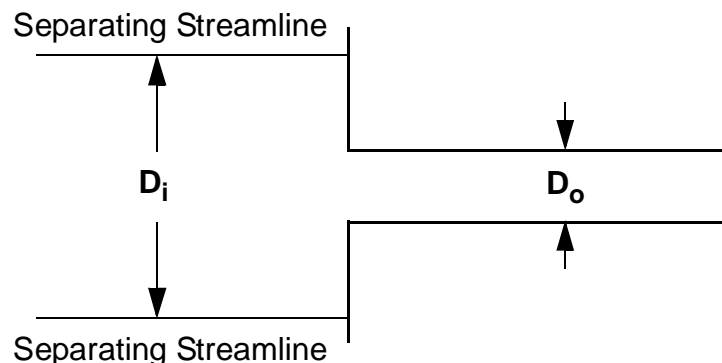


Figure 5.4. Illustration of a vena contracta.

Thermophoretic deposition is calculated separately for ceilings, walls, and floors because each may have a different surface temperature; thus an extra subscript is attached to the thermophoretic deposition velocities in Equations (5.51) through (5.53). Since thermophoretic deposition velocity can be negative and because the gravitational settling contribution is negative for a ceiling surface, the deposition velocities at ceilings, walls, and floors can have a net negative value. However, negative deposition velocities are set to 0 in VICTORIA, i.e., resuspension of deposited aerosols cannot occur as a result of the mechanisms described above. The removal rate in (5.16) is related to the net deposition velocities by the following expression:

$$R(m) = \frac{u_c A_c + u_w A_w + u_f A_f}{V_B} N(m) \quad (5.54)$$

5.7 Resuspension

Turbulent resuspension of deposited aerosol particles has been observed by many researchers and has been characterized by Wright et al. (Wright and Pattison, 1984; Wright et al., 1984) at the ORNL aerosol resuspension test (ART) facility. The resuspension model in VICTORIA is based on a power law curve fit to their data. The form is the same as the one used by Fromentin (1989) to correlate Swiss resuspension data and is also recommended by Reeks et al. (1988). The following relationships are used in VICTORIA:

$$F = 0 \text{ when } Re < 2300 \quad (5.55)$$

$$F = 0.05 \tilde{v}^2 t^{-1.25} \text{ when } Re > 2300 \quad (5.56)$$

where

- F = fractional rate of resuspension (1/s)
- \tilde{v} = friction velocity (m/s), as defined in Equation (5.32)
- t = time, measured from the point when Re first exceeds 2300 (s)

A number of simplifying assumptions are made in the VICTORIA implementation of the aerosol resuspension model, which include the following:

1. All aerosol particles are taken to have the same properties of adhesion to the substrate on which they are deposited. In other words, resuspension rates are independent of aerosol composition and of the properties of the substrate.
2. Once aerosol particles are deposited, they are taken to be immediately well mixed with previously deposited particles. Thus resuspended particles have the average composition of the surface layer from which they are removed.

Aerosol Processes

3. Resuspended particles have the same size distribution as the aerosol currently in the bulk gas of a node. An assumption of this type is needed because VICTORIA does not retain information about aerosol size distribution once deposition occurs.
4. Time in Equation (5.55) is measured from the point when the Reynolds number first exceeds 2300 in each node. Thus there is a single trigger for aerosol resuspension during a calculation.

The ART data, like most other resuspension data, are based on dry powders, i.e., aerosols that contain no liquid component during deposition or resuspension. The aerosols in the RCS during a severe accident are almost always composed of a mixture of liquid and solid, i.e., a slurry. Since it is doubtful that the resuspension model in VICTORIA well approximates resuspension of a slurry, the model has been made optional. The user should use this model only when dry-dust resuspension is being modeled, or as a means of estimating the sensitivity of predictions to the possibility of resuspension. The trigger for resuspension in the current model is when the Reynolds number first exceeds 2300 in a node.

5.8 Aerosol Size Distributions

Aerosol sources can be specified in the VICTORIA input for any node. The sources can be composed of one or more of the condensed-phase species in the VICTORIA database. Furthermore, the sources can be specified in a tabular manner as functions of time. Interpolation between tabulated values is linear. The primary restriction is that aerosol sources are taken to have log-normal size distributions, which are characterized by a mass median radius and a standard deviation.

Aerosol size distributions in the bulk gas of each node are treated numerically and are not assumed to have any specific distribution. However, it is sometimes useful to characterize the distribution in terms of a mean or median mass or diameter and of a standard deviation from that mean. There are several ways of characterizing distributions. Some of the more standard terms are defined below.

Mass median diameter is the particle diameter for which half of the total mass of aerosol particles has smaller diameters and the other half has larger diameters. Thus, the mass median diameter is defined by the following equations:

$$\frac{1}{2} = \frac{\int_0^{\hat{m}_m} N(m) dm}{\int_0^{\infty} N(m) dm} \quad (5.57)$$

$$\hat{m}_m = \frac{1}{6} \pi \rho_a \hat{d}_m^3 \quad (5.58)$$

where

$$\begin{aligned} \hat{m}_m &= \text{mass median mass (kg)} \\ N(m) &= \text{aerosol number concentration of particles of mass } m \text{ (1/m}^3\text{)} \\ dm &= \text{mass differential (kg)} \\ \hat{d}_m &= \text{mass median diameter of an equivalent spherical particle (m)} \end{aligned}$$

Part IV of this report describes the numerical techniques used in VICTORIA to solve for $N(m)$. Equations (5.56) and (5.57) are used to determine the mass median mass and diameter after the solution for $N(m)$ is obtained. Mass median diameter is probably the quantity most widely used to characterize the size of aerosol particles. In most cases, mass median diameters of the aerosols that form during a severe accident are approximately 10^{-6} m (1 μ).

The other term commonly used to characterize average particle size is the geometric mean diameter. Geometric mean diameter is defined as follows:

$$\ln(\bar{m}_g) = \frac{\int_0^{\infty} \ln(m) \frac{N(m)}{m} dm}{\int_0^{\infty} \frac{N(m)}{m} dm} \quad (5.59)$$

$$\bar{m}_g = \frac{1}{6} \pi \rho_a \bar{d}_g^3 \quad (5.60)$$

where

$$\begin{aligned} \bar{m}_g &= \text{geometric mean mass (kg)} \\ \bar{d}_g &= \text{geometric mean diameter (m)} \end{aligned}$$

Finally, the geometric standard deviation is defined as follows:

Aerosol Processes

$$[\ln(\sigma^3)]^2 = \frac{\int_0^{\infty} \left[\ln\left(\frac{m}{\bar{m}_m}\right) \right]^2 N(m) dm}{\int_0^{\infty} N(m) dm} \quad (5.61)$$

where

σ^3 = geometric standard deviation (dimensionless)

The values of the geometric standard deviation for aerosols that would be found in a severe accident are typically about 2.

Part II: Users Guide

6.0 Description of VICTORIA Input

6.1 Structure of Input File

VICTORIA input is broken up into three basic blocks. The first block is needed to initialize a calculation and must always be present at the top of the input file. This input is described in Section 6.2.

The second block of input data defines the static variables, i.e., those that are time independent and may not be redefined during a calculation. These input data immediately follow the initialization data and are organized by descriptors, which may occur in any order within the second block of data. A descriptor is the first line of each section of data. The descriptors and accompanying data (i.e., the sections of data) for this second block of input data are described in Section 6.3.

The second and third blocks of input data are separated by a PAUSE command, which is described in Section 6.4.

The third and final block of input data defines the variables that may be transient, either in the sense that they may depend explicitly on time or that they may be redefined during a calculation. These data are again organized by descriptors. Each descriptor defines a section of input. The order of these sections is somewhat but not entirely arbitrary. The descriptors and the accompanying data for the transient block of input data are described in Section 6.5.

The third block of input is terminated by an END command, which is described in Section 6.6. The input format for a restart run is described in Section 6.7.

The input reader in VICTORIA uses a free-field format and reads lines of input up to 80 characters in length. Either spaces or commas can be used to separate values on a single line of input. Many input variables have default values; these can be selected by leaving a blank space followed by a comma. Lines of input beginning with a "\$" (in the first space of the line) are interpreted as comments.

All data in the VICTORIA input are in Système International (SI) units. The specific units for each input variable are given in parentheses. Also, default values for all input variables are given below. Input data are illustrated for an input file that has been named `test.inp`. As the name would indicate, this input file is not intended to simulate any real plant accident or experiment; rather, it is intended as a comprehensive test of the VICTORIA capabilities. It is comprehensive in the sense that nearly all input options and modules are invoked. It is chosen here because it illustrates the main features of a VICTORIA input file.

Description of VICTORIA Input

The format that is used in the following sections is first to give small fragments of data interlaced with explanations of the meaning of each variable and the order in which the data must occur. Actual input data are indented and listed in a Courier font to distinguish them from the descriptions.

An illustration of the problem domain corresponding to the input data listed below is given in Figure 6.1. Again, this problem is defined merely for testing purposes and does not represent any reactor plant or experimental apparatus.

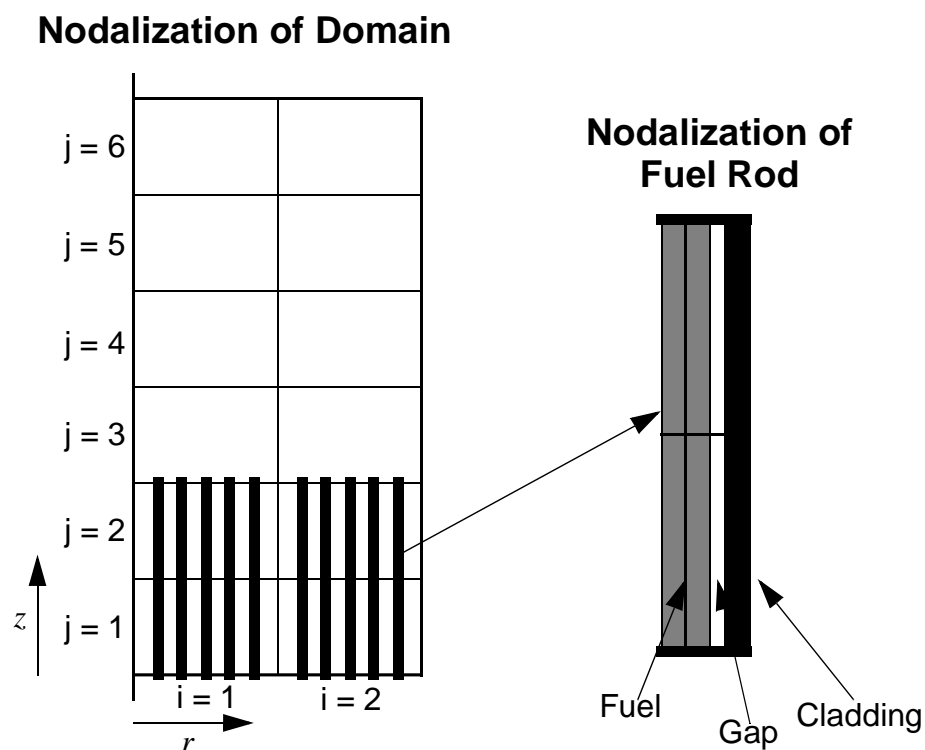


Figure 6.1. Nodalization and fuel subnodalization for the illustration in this chapter.

6.2 Initialization Data

The first block of data is used to initialize a calculation. The data in this block define very basic aspects of the calculation, such as which modules will be invoked and how the domain will be nodalized. This block of data is always required in a VICTORIA input file, although it is abbreviated for restart runs, as explained in Section 6.7.

Description of VICTORIA Input

```
$ Computer type:
  'SPARC 20'
$ Calculation Description:
  'Test Problem (NEB)'
```

The first two lines of input, disregarding comments, are basic descriptions of the job. The first line lists the computer type and the second describes the calculation that is being performed. The information in the second of these lines is printed at the top of each page of output.

```
$ restart
  0
```

A flag determines whether the current run is a restart from a previous calculation. The possible values of this flag and their meaning are:

- 0 the current run is not a restart
- 1 the current run is a restart

The input file format for a restart run is described in Section 6.7.

```
$ chemistry  aerosols  advection  release  decay  oxidation
    2          2        1          1        1        1
```

The next five flags govern the chemistry, aerosol, convection, fission product release, and decay heating modules of the VICTORIA code. The possible choices and their meanings are described below:

chemistry flag

- 0 chemistry modeling is inactive
- 1 chemistry modeling is active, a single condensed phase is treated
- 2 chemistry modeling is active, three condensed phases are treated

aerosol flag (this flag is referenced as iaero below)

- 0 aerosol modeling is inactive
- 1 aerosol modeling is active, resuspension modeling is inactive
- 2 aerosol and resuspension modeling are active

advection flag

- 0 advection modeling is inactive
- 1 advection modeling is active

release flag

- 0 fission product release modeling is inactive
- 1 fission product release modeling is active

Description of VICTORIA Input

decay heat flag

- 0 decay heat and structure heatup modeling are inactive
- 1 both decay heat and structure heatup modeling are active
- 2 decay heat modeling is active, structure heatup modeling is inactive

fuel oxidation flag

- 0 fuel oxidation modeling is inactive
- 1 fuel oxidation modeling is active

Differences in treatment of thermochemical equilibrium using the single- and three-phase assumptions are described in Subsection 4.1.3. The optional resuspension model is described in Section 5.7. The optional structure heatup model is described in Subsection 3.6.3.

There is at least one combination of the flags described above that is problematic. It is inadvisable for the user to attempt to treat chemistry but not aerosol behavior; if he did, vapors condensing in the bulk gas would have nowhere to deposit and masses would not be conserved. On the other hand, modeling aerosol behavior but not thermochemical equilibrium is a reasonable option.

```
$ axial ; radial ; fuel radial ; clad radial
6      2      2      1
```

The next line of data defines the nodalization of the domain and also a subnodalization used for fuel rods, if they are present. In this example, the nodalization consists of 6 axial levels, i.e., 6 nodes in the axial dimension z , and 2 radial rings, i.e., 2 nodes in the radial dimension r . Thus there are a total of 12 nodes. This nodalization is illustrated in Figure 6.1.

The notation used in VICTORIA for node numbering is a set of indices, (i,j) . In this notation, i numbers the nodes in the radial dimension and j numbers the nodes in the axial dimension. Each value of i corresponds to a radial ring; each value of j corresponds to an axial level. This usage is illustrated in Figure 6.1.

The subnodalization of the fuel rods defines the number of nodes in the radial dimension that represent the fuel pellets and the fuel cladding. In this example, there are 2 radial nodes to represent each fuel pellet and 1 node to represent the fuel cladding. Axial nodalization of fuel rods is defined in the same way as the domain. Nodalization of the fuel rods is illustrated in Figure 6.1. For rubble beds, the number of cladding nodes should be set to 0.

```
$ central radii
6*0.0
$ radial widths
6*0.7
```

Description of VICTORIA Input

```
6*0.3
$ axial heights
6*0.5
```

Several lines of data define the geometry of the domain. In this example, the central radii (m) are set to 0, indicating that the domain is cylindrical; annular domains can be defined by choosing these radii to be finite values. Six values are needed, one for each axial level, j . Here, the shorthand 6^* is used to indicate that the same value is repeated six times.

The next two lines of data indicate the radial widths (m) of each of the nodes. The first six values are for the central nodes, i.e., those closest to the z axis, and are ordered in the direction of the z axis. In other words, these values correspond to $i=1, j=1$ to $j=6$. The second six values are for the outer ring of nodes, i.e., those farther from the z axis, again ordered in the direction of the axis. These values correspond to $i=2, j=1$ to $j=6$. This ordering of data is used wherever a single value is needed for each node.

The final line of data contains the axial heights (m) of each element. One value is given for each axial location, again ordered in the direction of the axis. By implication, the axial dimensions of both rings are the same. This is a basic restriction of VICTORIA nodalizations.

6.3 Static Data

The second block of input data contains those that are static, i.e., not changing with time. This section describes these data. The second block of data is subdivided into eight sections, which describe the (1) fuel, (2) control rods, (3) structures, (4) mass transfer, (5) initial condition, (6) decay heat modeling, (7) aerosol modeling, and (8) special parameters that can be modified when necessary. Each section includes a descriptor as the first line, followed by a set of data. Some of these sections are optional and their order is arbitrary, so long as the entire block of data follows the initialization data described in Section 6.2 and precedes the PAUSE command, which is described in Section 6.4. Each section of data is described in one of the following subsections.

6.3.1 Fuel Data

The fuel data section of input is required if fission product releases are to be modeled, as determined by the release flag described in Section 6.2; otherwise, it can be omitted.

```
**FUELDATA
```

The above line is the descriptor for this section of input and must be the first line of the section.

Description of VICTORIA Input

```
$ pellet diam. ; gap thick. ; clad thick. ; He pressure ; frac theo dens
8.2E-03          1.6E-04          6.0E-04          2.5E+06          0.96
```

Following the descriptor is a line containing five parameters that define basic aspects of fuel rods. The first parameter defines the fuel pellet diameter, d (m). The second parameter defines the gap thickness, t_{gap} (m), i.e., the radial distance between the outer surface of the fuel and the inner surface of the cladding. The third parameter defines the cladding thickness, t_{clad} (m). Fuel rod geometry is illustrated in Figures 2.1 and 6.1. The fourth parameter defines the helium fill pressure of the fuel rod (Pa), which by convention corresponds to a temperature of 300 K. The final parameter on this line of input defines the fraction of theoretical density (dimensionless), which is just one minus the total fuel porosity, α , as discussed in Section 2.1. Each of these parameters affects fission product and uranium releases from fuel, which are described in Sections 2.1 and 2.5, respectively. When a debris bed is being modeled, the second, third, and fourth parameters on this line should be set to 0. Debris bed modeling is described in Section 2.2.

```
$ initial clad oxide level
0.0
```

The initial clad oxide level, x_{ox} , (dimensionless) represents the initial fraction of the zirconium in the fuel cladding that has oxidized before the start of the calculation. This parameter affects clad oxidation (Subsection 4.2.1), chemisorption of tellurium onto cladding (Subsection 4.2.2), and release of tin from the cladding (Section 2.6).

```
$ number of fuel rods per node
2*5, 4*0
2*5, 4*0
```

The number of fuel rods per node is given in the same order as described above. The location of the fuel rods for this example is illustrated in Figure 6.1.

```
$ Permeabilities
$ fuel      gap(radial,axial)  cladding  fuel layer
1.e-15      1.e-13  1.e-13      1.e-14      1.e-13
```

Treatment of porous flow in the fuel rods is described in Section 2.1. Input data consists of the radial permeability of the fuel pellets, κ in Subsection 2.1.2, radial and axial permeabilities in the gap, κ_r and κ_z in Subsection 2.1.3, the radial permeability of the cladding, κ in Subsection 2.1.4, and the radial permeability of the boundary layer external to the fuel rod, κ in Section 3.3.

Permeabilities are expressed in units of m^2 . Porous flows in the gap and fuel boundary layer actually represent laminar flows, so the permeabilities in these two subregions should be relatively higher than those in the other subregions. The primary reason for including the porous flow model in the fuel is to alleviate large pressure differentials

Description of VICTORIA Input

between the gases in the fuel pores and the gases in the coolant channel, which can exist when diffusion is the sole transport mechanism. The developers have found that fission product release rates generally are not sensitive to the choice of permeability, so long as reasonable values are chosen. Section 2.1 discusses this point in more detail.

```
$ Number of Elements in the Fuel grains
15
```

The next input parameter is the number of elements to be modeled in the fuel grains, including the fission products, uranium, and oxygen. Even though the VICTORIA database contains 26 elements, not all of them are found in significant quantity as fission products. Typically, 15 or fewer elements are modeled. The initial inventory of these elements and parameters to describe their diffusivities in the fuel grains are contained in the next set of input data.

```
$ Fuel grain inventories and diffusion coefficients
$ element
  'U'
$ dzero ; theta
      '      '
37.79 37.79
37.79 37.79
37.79 37.79
37.79 37.79
$ element
  'O'
$ dzero ; theta
      '      '
76.3358 76.3358
76.3358 76.3358
76.3358 76.3358
76.3358 76.3358
$ element
  'Cs'
$ dzero ; theta
      '      '
0.118 0.118
0.118 0.118
0.118 0.118
0.118 0.118
$ element
  'Ba'
$ dzero ; theta
      '      '
6.311e-2 6.311e-2
6.311e-2 6.311e-2
6.311e-2 6.311e-2
6.311e-2 6.311e-2
$ element
```

Description of VICTORIA Input

```

'I'
$ dzero ; theta
    '
    0.0091 0.0091
    0.0091 0.0091
    0.0091 0.0091
    0.0091 0.0091
$ element
'Sr'
$ dzero ; theta
    '
    0.064 0.064
    0.064 0.064
    0.064 0.064
    0.064 0.064
$ element
'Zr'
$ dzero ; theta
    '
    0.228 0.228
    0.228 0.228
    0.228 0.228
    0.228 0.228
$ element
'Sn'
$ dzero ; theta
    '
    0.0024 0.0024
    0.0024 0.0024
    0.0024 0.0024
    0.0024 0.0024
$ element
'Te'
$ dzero ; theta
    '
    0.019 0.019
    0.019 0.019
    0.019 0.019
    0.019 0.019
$ element
'Kr'
$ dzero ; theta
    '
    0.026 0.026
    0.026 0.026
    0.026 0.026
    0.026 0.026
$ element
'Xe'
$ dzero ; theta
    '

```


Description of VICTORIA Input

```
0.228    0.228
0.228    0.228
0.228    0.228
0.228    0.228
$ element
'Mo'
$ dzero ; theta
      '      '
0.188    0.188
0.188    0.188
0.188    0.188
0.188    0.188
$ element
'Ru'
$ dzero ; theta
      '      '
0.132    0.132
0.132    0.132
0.132    0.132
0.132    0.132
$ element
'Sb'
$ dzero ; theta
      '      '
0.0009   0.0009
0.0009   0.0009
0.0009   0.0009
0.0009   0.0009
$ element
'Eu'
$ dzero ; theta
      '      '
0.0057   0.0057
0.0057   0.0057
0.0057   0.0057
0.0057   0.0057
```

The format in this section of data is to list the name of the element on the first line, the grain diffusion coefficients on the second line, and initial inventories in the fuel grains on the subsequent lines. The name of the element is read as alphanumeric data, and must be in quotes on some machines; thus, **it is good practice to place quotes around all alphanumeric data, even if this is not required on the machine you are using.**

The grain diffusion coefficients, $D_0(i)$ and $\theta(i)$, correspond to Equation (2.10) and are given in units of m^2/s and K, respectively. In this example, default values for these diffusion coefficients are selected. Finally, the inventory of each element in the fuel is given in units of $\text{kg-mol}/\text{m}^3$. The ordering of these data is first over the nodes in the subnodalization of the fuel, then over the axial levels (j), and finally over the radial rings (i). These data are provided only for the nodes that contain fuel. Thus the first line of data corre-

Description of VICTORIA Input

sponds to the two fuel nodes, ordered outward from the fuel centerline, in node $i=1, j=1$. The following lines of data correspond respectively to nodes $i=1, j=2$; $i=2, j=1$; and $i=2, j=2$.

```
$ grain diameters
    2*1.0e-5
    2*1.0e-5
    2*1.0e-5
    2*1.0e-5
```

The final set of data in this section describes the grain diameters, a (m); in this example, all grain diameters are $10\text{ }\mu$. The ordering of data is the same as that described above for the fission product inventories.

6.3.2 Control Rod Data

This section of data provides information on silver/indium/cadmium control rods, if they are to be modeled; if they are not to be modeled, this section of data would normally be omitted in the input file.

```
**CORODATA
```

The above line is the descriptor for this section of input and must be the first line of the section.

```
$ absorber          control rod cladding
$ diam.    length   int. diam.  ext. diam.  length
    8.66e-3  0.90      8.7e-3     9.7e-3     1.00
```

The absorber diameter and length define the dimensions of the control rod alloy in its original, solid state. The second set of dimension are for the control rod cladding. All of these dimensions are in meters.

```
$ mass fraction      helium fill
$ Ag    In    Cd    pressure (Pa)
    0.80  0.15  0.05  1.5e5
```

The next set of parameters defines the composition of the interior of the control rod. The composition of the alloy is expressed in terms of the mass fractions of silver, indium, and cadmium. The control rod is also charged with helium. The fill pressure is measured at 273 K and is in units of pascals.

```
$ number of control rods
    2*1,4*0
    2*1,4*0
```

Description of VICTORIA Input

The final set of data defines the number of control rods in each node. These data are in the usual order, as described in Section 6.2.

6.3.3 Structure Data

The section of input data describing structures is required for all VICTORIA calculations.

```
**STRUDATA
```

The above line is the descriptor for this section of input and must be the first line of the section.

```
$ Flags for inner rings
$ flow irregularity flags
  3*0 3 4 2
$ node 4 steam separator information
$ tube length tube radius vane angle (rad)
  0.05         0.15         0.52
$ node 5 steam dryer information
$ no. of bends tube angle (rad) bend spacing
  5            1.04         1.5
$ node 6 abrupt contraction information
$ inlet diam. exit diam
  0.7          0.35
$ Flags for outer rings
$ flow irregularity flags
  1 2*0 3 4 1
$ node 4 steam separator information
$ tube length tube radius vane angle (rad)
  0.05         0.15         0.52
$ node 5 steam dryer information
$ no. of bends bend angle (rad) bend spacing
  5            1.04         1.5
```

The first set of data in this section describes flow irregularities. A set of flags determines which flow irregularities are found in each node. These flags are given first for the central ring, corresponding to $i = 0$. The flags have the following definitions:

- 0 no flow irregularity, i.e., flow is through a pipe or annulus
- 1 flow is through a 90° pipe bend
- 2 flow is through a sudden contraction
- 3 flow is through an upcomer, cyclone-type steam separator
- 4 flow is through a chevron-type steam dryer
- 5 flow is through a vena contracta

The models for inertial deposition of aerosols due to these flow irregularities are described in Subsection 5.6.5. Only one flow irregularity can be treated in each node;

Description of VICTORIA Input

thus, the nodalization must be on a fine enough scale so that no more than one flow irregularity need be treated within a single node.

When the flow irregularity flag is set to 2, 3, 4, or 5, additional input data are needed. In the inner ring of nodes, additional data are needed for nodes 4, 5, and 6. Following this is a similar set of data for the six nodes in the outer ring.

The additional data needed for a sudden contraction (flag = 2) are the inlet and exit diameters (m); for a steam separator (flag = 3), they are the vortex tube length (m) and diameter (m), and the vane angle (rad); for a steam dryer (flag = 4), they are the number of bends (dimensionless), the bend angle (rad), and the perpendicular spacing between the chevron vanes (m); and for a vena contracta (flag = 5), they are the inlet and exit diameters (m). These parameters are described further in Subsection 5.6.5.

```
$ settling parameters
6*-1.0
6*-1.0
```

Settling parameters are connected with internodal gravitational settling, as described in Section 3.5. Three settling parameters define the direction of gravitational acceleration: When the direction of gravitational acceleration and the z axis are diametrically opposed, this parameter should be set to -1; when the directions are the same, this parameter should be set to +1; when they are orthogonal, it should be set to 0. In general, the settling parameter is the cosine of the angle between the z axis and the direction of gravitational acceleration.

```
$ axial flow areas
2*1.4921,3*1.5394,0.3848
2*1.5549,3*1.6022,0.0
```

Axial flow areas (m^2) characterize the area that is open to flow in the axial direction. In this example, the nodes at the first two axial levels have smaller surface areas than those above because the areas of the fuel and control rods and supporting structures have been subtracted. When a node represents a region that is irregular, these areas generally should represent the upper boundary of the node, as defined by the direction of the z axis. Further guidance on selecting values to represent flow areas is given in Part IV of this report.

```
$ radial flow areas
6*2.1991
6*0.0
```

Radial flow areas (m^2) are analogous to axial flow areas. They characterize the area open to flow in the radial dimension and generally characterize the outer surface of the node.

Description of VICTORIA Input

```
$ hydraulic diameters
2*0.3630,4*1.4
2*0.2757,4*1.02
```

Hydraulic diameters (m) are defined in the usual way. For a cylindrical pipe, the hydraulic diameter is simply the pipe diameter. For noncylindrical regions, hydraulic diameter is usually defined as four times the area divided by the wetted perimeter.

```
$ floor area in node
1.1545,5*0.0
1.6022,5*0.0
$ wall area in node
6*0.1
6*3.1416
$ ceiling area in node
5*0.0,1.1545
5*0.0,1.6022
```

Floor, wall, and ceiling areas (m²) define the surface areas for aerosol deposition, as described in Section 3.5 and Subsection 5.6.6.

```
$ structure identification flags
6*0
1,2,3,4,5,6
```

Structure identification flags define the composition of a surface. The possible choices for this flag are the following:

- 0 inert surface
- 1 Zircaloy-4 surface
- 2 Inconel-600 surface
- 3 stainless steel-304 surface
- 4 oxidized Inconel-600 surface
- 5 oxidized stainless steel-304 surface
- 6 zirconia surface

The choice of surface affects modeling of chemisorption, as described in Subsection 4.2.2.

6.3.4 Mass Transfer Data

All mass transfer data have default values, and so this input data section is optional. Models and default parameters are described in Sections 3.2 and 3.3. This section of data provides the option to override the defaults and is thus useful for sensitivity studies. The values provided in this example are identical to the defaults, and so can be used as a starting point for sensitivity studies.

Description of VICTORIA Input

```
**LAYRDATA
```

The above line is the descriptor for this section of input and must be the first line of the section.

```
$ Sherwood number  
0.0
```

Ordinarily, the Sherwood number (dimensionless) is calculated according to the correlations set out in Sections 3.2 and 3.3. However, the user can override these correlations and set the Sherwood number explicitly. If this value is omitted (using a comma) or set equal to zero, the normal correlations are used to determine mass transfer.

```
$ Boundary layer multipliers  
$ fuel      structure  
1.0        1.0
```

Ordinarily, diffusion layer thickness, as set out in Equations (3.6) and (3.7), subject to a maximum, as expressed Equation (3.9), is used to define the fuel and structure layer subregions, which are illustrated in Figure 3.1 and described in Section 3.2. The default layer thicknesses for the fuel and structure subregions can be modified with the above multipliers (dimensionless). When these multipliers are both equal to unity, the defaults are used. When they are greater than unity, the layer thicknesses are proportionally greater than the defaults; conversely, when they are smaller than unity, the layer thicknesses are proportionally smaller than the defaults. The layer thickness for the control rod subregion is taken to have the same value as the fuel layer thickness.

```
$ Fraction of maximum thickness  
0.5
```

A parameter (dimensionless) defines the fraction of the maximum layer thickness that is allowed, as defined in Equation (3.9). This fraction is normally one-half, i.e., the fuel and structural layer thicknesses are permitted to be as much as one-half of their maximum values. Maximum values are calculated from geometrical constraints, as described in Section 3.2.

```
$ multipliers for mass transfer boundary layer thicknesses  
$ fuel      structure  
1.0        1.0
```

An alternative to specifying the Sherwood number, as described above, is to modify the multipliers for the fuel and structural boundary-layer thicknesses, which normally have values of unity. Increasing or decreasing these values increases or decreases the layer thicknesses for the two subregions, respectively. Increasing the boundary layer thickness decreases the mass transfer coefficient, as defined in Equation (3.16).

Description of VICTORIA Input

6.3.5 Initial Condition Data

Initial condition data are required for all VICTORIA calculations. These data specify the gases that are present in the problem domain at the start of the calculation.

```
**CONTDATA
```

The above line is the descriptor for this section of input and must be the first line of the section.

```
$ initial species present  
1
```

The second line indicates the number of vapor-phase species that are present at the start of a calculation. The input reader expects to find the following set of data once for each species.

```
$ species name  
  'H2Og'  
$ species mass concentrations  
  6*3.2475  
  6*3.2475
```

The first line is an alphanumeric string that specifies the name of the vapor-phase species. In this example, only steam is present at the start of the calculation. The subsequent two lines of data indicate, in the usual order, the initial mass concentrations (kg/m³) of the vapor-phase species in each node. These data should be consistent with the initial pressure and temperature data that are described below, i.e., the initial partial pressures, calculated by the ideal gas law, should sum to the total pressure.

6.3.6 Decay Heat Data

Decay heat data are required when the decay heat module is active, as determined by the flag described in Section 6.2. However, when this flag is set to 2, the data that define thermal properties are not used.

```
**DECAY
```

The above line is the descriptor for this section of input and must be the first line of the section.

```
$ decay heat initialization flag  
2
```

The decay heat initialization flag determines how a normalization for the amount of decay heat per unit mass of each fission product is calculated, as described in Section 3.6. This flag can have the following values:

Description of VICTORIA Input

- 1 normalization determined from data included below
- 2 normalization determined from fission product inventory in fuel

If fuel is present in the calculation, most commonly the user would set the flag to 2 and use the masses of fission products in the fuel as the basis for the normalization. In some cases, decay heating calculations are performed when there is no fuel present; in these cases, fission products are introduced as vapor or aerosol sources. Setting the initialization flag to 1 requires additional data to specify the fission product inventory from which decay heats are to be calculated. These additional data are described below.

```
$ insulation    time since  reactor power (kW)
$ temperature   scram
    300.         0.         10.
```

The values on this line of input indicate the temperature (K) of the insulation, T_I , outside the surface of the structure. This value is used to calculate structural heatup, as described in Subsection 3.6.3. In some cases, the time of reactor scram or shutdown may not coincide with time equals zero in the VICTORIA calculation. When this is so, the value of "time since scram" (s) indicates the elapsed time between scram and the point when time equals zero in the VICTORIA calculation. To eliminate any confusion, the best practice is simply to measure time from the point when scram occurs and set this parameter to zero. The third value on this line of input is the total thermal power of the reactor (kW) just prior to scram, Q_{Tot} . This value is used to determine the decay power produced by each fission product element following scram.

```
$ structure failure temperature
    2500.
```

A structure is assumed to fail catastrophically when it reaches the prescribed structure failure temperature (K). This criterion is applied only to structures whose temperatures are being calculated, as determined by the set of flags described below. When a structure fails, the VICTORIA calculation is terminated. If the user wishes to avoid termination of a calculation due to such a failure, then this parameter should be set artificially high, as is done in this example.

```
$ heatup flags at boundary
$ inner upper bottom outer
    6*0    2*1    2*0    6*1
```

The structural heatup modeling described in Subsection 3.6.3 is appropriate only at the exterior boundaries of a problem domain. A set of flags determines the nodes for which decay heating modeling will be invoked. The meaning of these flags is as follows:

- 0 indicates that decay heating is not to be calculated for structures in this node
- 1 indicates that decay heating is to be calculated for structures in this node

Description of VICTORIA Input

The ordering of this data is as follows: the first set of flags is for the inner surface of the problem domain, corresponding to $i = 1$, and is numbered from $j = 1$ to $j = j_{\max}$; the second set of values is for the upper surface of the domain, corresponding to $j = j_{\max}$, and is numbered from $i = 1$ to $i = i_{\max}$; the third set of values is for the bottom surface of the domain, corresponding to $j = 1$, and is numbered from $i = 1$ to $i = i_{\max}$; the fourth and final set of values is for the outer surface of the domain, $i = i_{\max}$, and is numbered from $j = 1$ to $j = j_{\max}$. Unless the problem domain is annular, the flags for the inner surface of the domain should be set to 0; otherwise the surfaces would be at the axis of symmetry and would have no area. In this example, i_{\max} is 2 and j_{\max} is 6 and decay heating is calculated at the top and outer boundaries of the problem domain.

```
$ thicknesses of pipe walls (m)
16*0.005
```

Thicknesses (m) of pipe walls are specified in the same order as the heatup flags described above. These values are used only for the nodes where the heatup flag is set to 1.

```
$ thermal conductivity of the insulation (W/m/K)
16*0.001
```

The next set of values specifies the thermal conductivities (W/m·K) of any insulation that may be present at the exterior of a pipe or surface. When no insulation is present, these values should indicate the thermal conductivity of a thermal boundary layer outside the surface. These values should not be 0 for any of the nodes for which structural heatup is being calculated.

```
$ thicknesses of the insulation (m)
18*0.05
```

The final set of parameters in this section of data specifies the thickness of insulation on the external surface of a pipe or structure. If no insulation is present, these parameters should be chosen to represent the thickness of the thermal boundary layer. These values should not be 0 for any of the nodes for which structural heatup is being calculated.

The following set of data must be included when the decay heat initialization flag is set to 1, but otherwise must be omitted:

```
$ number of elements in fuel
13
$ initial element masses in fuel
'Ba'
1.789E-01
'Cs'
4.158E-01
'I'
6.682E-02
```

Description of VICTORIA Input

```
'Mo'  
3.961E-01  
'Ru'  
2.610E-01  
'Sr'  
1.203E-01  
'Te'  
8.959E-02  
'U'  
9.369E+00  
'Zr'  
4.567E-01  
'Sb'  
2.012E-03  
'Eu'  
1.569E-02  
'Kr'  
4.889E-02  
'Xe'  
5.829E-01
```

In this example, there are 13 fission products in the fuel; by assumption, any that are not defined to be in the fuel do not contribute to decay heating. For each fuel element, a pair of lines is required. The first gives the name of the element; the second gives the fission product inventory of the fuel that acted as the source of the fission products. If this fuel represents a fraction of the fuel that was originally in a reactor core, then the same fraction of the full reactor power prior to scram should be used above.

6.3.7 Aerosol Data

A section of aerosol data must be included in VICTORIA calculations if aerosol modeling is active. The parameters included in this example are the default values that would be obtained if they had been left blank.

```
**AERODATA
```

The above line is the descriptor for this section of input and must be the first line of the section.

```
$ Definition of collocation points  
$   ncoll      ;   spacing  
    0           10.  
$   mlower     ;   mupper  
    1.e-22      1.e-11
```

The next set of data defines the collocation points used for numerical representation of the aerosol size distribution, as described in Part IV of this report. The default values are

Description of VICTORIA Input

that the number of collocation points is zero, the spacing between collocation points is a factor of 10, the smallest aerosol size represented has a mass of 10^{-22} kg, and the largest aerosol size represented has a mass of 10^{-11} kg.

One of the values used to define the collocation points is redundant. In this example, by defining the number of collocation points to be 0, this number is recalculated to be 12; if the number of collocation points had been set to a finite value, then the spacing would have been recalculated to be consistent with the other data.

```
$ element number
2
```

The element number indicates the type of finite-element basis function to be used in the representation of aerosol size distribution. The allowable values indicate the following finite-element basis functions:

- 1 piecewise-constant
- 2 piecewise-linear
- 3 piecewise-cubic

The default value of 2, indicating piecewise linear basis functions, is recommended for most calculations. A choice of 1 would give lower-order accuracy and a choice of 3 would give higher-order accuracy than the default value of 2. Computational costs increase as accuracy increases.

```
$ Tolerance specification
$ eps      ; maxtrys
1.e-6      10
```

These tolerance specifications are numerical parameters that are used to control time integration of Equation (5.20). The first value determines the relative error that is allowed at each time step (dimensionless). Values for this parameter should be in the range of 10^{-3} to 10^{-8} . The second parameter determines the maximum number of attempts that will be made to perform the time integration before quitting and issuing an error message.

```
$ Aerosol physics data
$ cshpfctr dshpfctr stickeff
1.0        1.0        1.0
```

This line of data defines the collisional and dynamic shape factors, χ_c and χ_d , respectively, and the particle-to-particle sticking efficiency, ϵ_s . These parameters are dimensionless and are defined in Subsections 5.2.3 and 5.5.1.

```
$ k1      k2      k3
1.25      0.41      0.88
```

Description of VICTORIA Input

These are the dimensionless empirical coefficients, k_1 , k_2 , and k_3 , used to define Cunningham's slip correction factor in Equation (5.18).

```
$ cmbrock  csbrock  ctbrock
    1.14      1.17      2.18
```

The final group of data in this section consists of the parameters used to determine thermophoretic deposition rates in the Brock model given in Equation (5.42). These are the momentum accommodation coefficient (dimensionless), C_m , the thermal slip coefficient (dimensionless), C_s , and the thermal accommodation coefficient (dimensionless), C_t .

6.3.8 Namelist Parameters

The namelist section of input data is not normally included in a VICTORIA calculation. It is provided as a means of gaining access to variables that are not normally modified.

****NAMELIST**

The above line is the descriptor for this section of input and must be the first line of the section. The syntax required to modify a namelist parameter in the static block of data is as follows:

```
$namest
  fulthk = 0.
  strthk = 0.
  jacksn = 1
  crdthk = 1.75e-4
  crdhmx = 0.35
  crdtim = 10.
$end
```

Notice that the dollar signs must be indented one space to distinguish these lines from comments. The values given above are the defaults that would be obtained if the namelist section of input were omitted. Only those namelist parameters that are to be modified from the default value need be included in this section of data; those that are not included will retain their default values. The above variables have the following meanings:

fulthk	Surface layer thickness (m) of the fuel grains that is included in fuel pore chemistry calculations [0]. The default for this parameter in VICTORIA-92 was $5 \cdot 10^{-9}$ m.
strthk	Surface layer thickness (m) of structures that is included in chemistry calculations for structure layer subregions [0]. The default for this parameter in VICTORIA-92 was $5 \cdot 10^{-9}$ m.
jacksn	A flag (dimensionless) that determines whether the Jackson's thermochemical data for hydroxides are used [1]. This flag can have the following values:

Description of VICTORIA Input

- 0 Jackson's thermochemical data are used to compute the concentrations of these hydroxide species
 - 1 Jackson's thermochemical data are not used and the concentrations of these species are set to zero
- The default value of this parameter in VICTORIA-92 was 0.
- crdthk** Thickness (m) of the layer of control rod alloy, δ_{CR} , that forms on the surface below the failure point [$1.75 \cdot 10^{-4}$], as described in Section 2.4. The default value in VICTORIA-92 was the same.
- crdhmx** Maximum fraction (dimensionless) of the thickness of the control rod layer subregion that can be occupied by control rod alloy [0.35]. The default value in VICTORIA-92 was the same.
- crdtim** Time offset, t_o , (s) used in Equation (2.34) [10]. The default value in VICTORIA-92 was the same.
- rlermx** The maximum relative error (%) between the input and calculated pressure of a node that is allowed without termination [50].

6.4 Pause Command

****PAUSE**

This line must be used to separate static data, as described above, from transient data, as described below.

6.5 Transient Data

The third and final block of input data consists of those that are transient, i.e., changing with time. The third block of data is subdivided into eight sections, which describe (1) chemistry modeling, (2) fuel temperatures, (3) thermal hydraulics, (4) mass sources, (5) special parameters, (6) subdomain coupling, (7) time stepping and output of data, and (8) start of a calculation. Some of these sections are optional and their order is fairly flexible; however, this entire block of data must follow the PAUSE command described in Section 6.4. Each section of data is described in one of the following subsections.

6.5.1 Chemistry Data

The parameters defined in this section of data do not have defaults, and thus this section is required in all VICTORIA calculations.

****TDEPCHEM**

The above line is the descriptor for this section of input and must be the first line of the section.

```
$ max chem. iter. ; convergence criterion ; max cyclic Newton iter.  
200                1.e-8                20
```

Description of VICTORIA Input

The subsequent line prescribes three parameters that affect the numerical procedures for determining equilibrium thermochemistry. The first of these parameters determines the maximum number of iterations (dimensionless) to be allowed. The second parameter determines the convergence criterion (dimensionless), which is in terms of the maximum relative error of the vapor-phase elemental concentrations. In other words, for a solution to be accepted as representing thermochemical equilibrium, the maximum change during an iteration of any of the elemental vapor-phase concentrations cannot be more than 10^{-8} of its value. The final parameter on this line is the maximum number of cyclic Newton iterations that will be attempted before performing a Newton-Raphson iteration step. The numerical procedure used to solve for thermochemical equilibrium is described in more detail in Part IV of this report.

```
$ gas diff. (0,1,2); frozen chem on/off (1/0); temp threshold (K)
1                      0                      1000.
```

The final line in this section of input data prescribes the method that is used for determining gas-phase diffusivities (as described in Section 2.1) and whether the “frozen chemistry” model will be invoked (as described in Subsection 4.2.3). The first parameter is a flag that can have the following values:

- 0 gas-phase diffusivities are calculated for diffusion in a steam/hydrogen/helium mixture, both in the fuel and the bulk gas
- 1 gas-phase diffusivities are calculated for diffusion in a steam/hydrogen/helium mixture in the fuel, but for diffusion in the actual mixture of gases in the bulk gas
- 2 gas-phase diffusivities are determined for diffusion in the actual mixture of gases, both in the fuel and the bulk gas

The second parameter is a flag that determines whether the frozen chemistry model will be invoked as follows:

- 0 frozen chemistry will not be invoked
- 1 frozen chemistry will be invoked for regions where the temperature falls below the prescribed threshold value

The final parameter on this line determines the threshold value (K) that will be used for the frozen chemistry model. For temperatures above this threshold, the normal equilibrium thermochemistry model will be used; for temperatures below this threshold, the frozen chemistry model will be invoked.

6.5.2 Thermal Data for Fuel

This section of input can be omitted when fuel is not being modeled; it must be present when fuel is being modeled.

```
**TDEPFUEL
```

Description of VICTORIA Input

The above line is the descriptor for this section of input and must be the first line of the section.

```
$ fuel temperature interpolation flag
1.0
```

The fuel temperature interpolation flag determines how radial temperature gradients within fuel pellets are interpolated. The two following options are allowed:

- 1 temperature interpolation is linear
- 2 temperature interpolation is quadratic

The first option would normally be used during periods when a reactor has been shut down or scrammed; the second option would normally be used during operation of a reactor. In both interpolation schemes, the thermal profile is determined by centerline and surface temperatures that are defined below. In addition, for the parabolic interpolation scheme, the thermal profile is taken to have a zero gradient at the fuel-rod centerline.

```
$ number of time values for temperature arrays
15
```

Thermal data for the fuel are interpolated from data tables included below. The above parameter specifies the number of time values in the tables. At a minimum, two time values should be specified because VICTORIA expects to perform interpolations.

```
$ time values (s) for fuel temperatures
0.    50.    150.    200.    250.    300.    350.    400.
900.  1000.  1050.  1100.  1150.  1200.  1250.
```

These lines of data contain the time values (s) for the tabular thermal data included below. The number of time values is specified by the parameter on the preceding line, which in this case is 15.

```
$ fuel center-line temperatures (K)
$ inner ring, i=1
$ j=1
1050.0  1750.0  1750.0  1750.0  2050.0  2050.0  2250.0  2550.0
2550.0  1050.0  1050.0  1050.0  1050.0  1050.0  1050.0
$ j=2
1050.0  1650.0  1650.0  1650.0  1950.0  1950.0  2150.0  2450.0
2450.0  1050.0  1050.0  1050.0  1050.0  1050.0  1050.0
$ j=3
15*0.0
$ j=4
15*0.0
$ j=5
15*0.0
$ j=6
```

Description of VICTORIA Input

```
15*0.0
$ outer ring, i=2
$ j=1
1050.0 1250.0 1250.0 1250.0 1550.0 1550.0 1750.0 2050.0
2050.0 1050.0 1050.0 1050.0 1050.0 1050.0 1050.0
$ j=2
1050.0 1150.0 1150.0 1150.0 1450.0 1450.0 1650.0 1950.0
1950.0 1050.0 1050.0 1050.0 1050.0 1050.0 1050.0
$ j=3
15*0.0
$ j=4
15*0.0
$ j=5
15*0.0
$ j=6
15*0.0
```

Fuel centerline temperatures (K) are prescribed in the following order; this same order is used for most of the transient data described below. On each line (or set of lines if the data do not fit on one line) are the values for a single node at each of the time values given above. In this example, there are 15 temperatures corresponding to the 15 time values specified above. Since these data do not all fit on a single line, two lines are used. The data are given for nodes ordered in the same way as described for the static data, i.e., in the central ring from bottom to top, then in the second ring from bottom to top, etc. Because only the bottom two axial levels contain fuel, the values for the upper levels have no effect on the results; in this case they are set to zero.

```
$ fuel surface temperatures (K)
$ inner ring, i=1
$ j=1
1025.0 1725.0 1725.0 1725.0 2025.0 2025.0 2225.0 2525.0
2525.0 1025.0 1025.0 1025.0 1025.0 1025.0 1025.0
$ j=2
1025.0 1625.0 1625.0 1625.0 1925.0 1925.0 2125.0 2425.0
2425.0 1025.0 1025.0 1025.0 1025.0 1025.0 1025.0
$ j=3
15*0.0
$ j=4
15*0.0
$ j=5
15*0.0
$ j=6
15*0.0
$ outer ring, i=2
$ j=1
1025.0 1225.0 1225.0 1225.0 1525.0 1525.0 1725.0 2025.0
2025.0 1025.0 1025.0 1025.0 1025.0 1025.0 1025.0
$ j=2
1025.0 1125.0 1125.0 1125.0 1425.0 1425.0 1625.0 1925.0
```


Description of VICTORIA Input

```
1925.0 1025.0 1025.0 1025.0 1025.0 1025.0 1025.0
$ j=3
15*0.0
$ j=4
15*0.0
$ j=5
15*0.0
$ j=6
15*0.0
```

Following the fuel centerline temperatures (K), the fuel surface temperatures are given in the same order.

```
$ Cladding temperatures (K)
1000.0 1700.0 1700.0 1700.0 2000.0 2000.0 2200.0 2500.0
2500.0 1000.0 1000.0 1000.0 1000.0 1000.0 1000.0
1000.0 1600.0 1600.0 1600.0 1900.0 1900.0 2100.0 2400.0
2400.0 1000.0 1000.0 1000.0 1000.0 1000.0 1000.0
15*0.0
15*0.0
15*0.0
15*0.0
$
1000.0 1200.0 1200.0 1200.0 1500.0 1500.0 1700.0 2000.0
2000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1000.0
1000.0 1100.0 1100.0 1100.0 1400.0 1400.0 1600.0 1900.0
1900.0 1000.0 1000.0 1000.0 1000.0 1000.0 1000.0
15*0.0
15*0.0
15*0.0
15*0.0
```

Finally, the cladding temperatures (K) are given in the same order as the fuel temperatures.

```
$ cladding failure temperature (K)
2000.0
$ cladding interconnected porosity when fully oxidized
0.05
$ cladding melt temperature
2100.0
```

The final three parameters describe conditions for cladding failure. The first parameter determines the temperature (K) for which the cladding first fails, T_{fail} . The appropriate cladding failure temperature is usually determined from a thermal-hydraulics code. The second parameter is used when the cladding fails from excessive oxidation, as described in Subsection 2.1.4. This parameter specifies the interconnected porosity of the fuel cladding upon failure from oxidation, β_{ox} (dimensionless). The final parameter provides the

Description of VICTORIA Input

temperature for which the cladding melts or is completely removed, T_{melt} (K). Above this temperature, the fuel is treated as a rubble bed, as described in Section 2.2.

6.5.3 Thermal-Hydraulic Data for Bulk Gas and Structures

This section of input data is required for all VICTORIA calculations and contains thermal-hydraulic data for the bulk gas and structures. This section should follow the TDEPFUEL section if that section is included in the input file. The format of data in this section is very similar to that used in the TDEPFUEL section.

****TDEPSTRU**

The above line is the descriptor for this section of input and must be the first line of the section. The following line of data should be included when the input file contains no TDEPFUEL section; otherwise it should be omitted.

\$ number of time values for temperatures
15

This line specifies the number of time values in the following data tables. When the TDEPFUEL section of data is included, this parameter is defined there.

\$ time values (s) for gas temperatures
0. 50. 150. 200. 250. 300. 350. 400.
900. 1000. 1050. 1100. 1150. 1200. 1250.

These time values (s) correspond to the gas temperatures in the following data table. The time values do not need to be the same as those used in the TDEPFUEL section of input; however, the same number of values must be included.

\$ gas temperatures (K)

1000.0	1600.0	1600.0	1600.0	1900.0	1900.0	2100.0	2400.0
2400.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1500.0	1500.0	1500.0	1800.0	1800.0	2000.0	2300.0
2300.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1400.0	1400.0	1400.0	1700.0	1700.0	1900.0	2200.0
2200.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1300.0	1300.0	1300.0	1600.0	1600.0	1800.0	2100.0
2100.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1200.0	1200.0	1200.0	1500.0	1500.0	1700.0	2000.0
2000.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1100.0	1100.0	1100.0	1400.0	1400.0	1600.0	1900.0
1900.0	750.0	750.0	750.0	750.0	750.0	750.0	
\$							
1000.0	1100.0	1100.0	1100.0	1400.0	1400.0	1600.0	1900.0
1900.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1000.0	1000.0	1000.0	1300.0	1300.0	1500.0	1800.0
1800.0	750.0	750.0	750.0	750.0	750.0	750.0	

Description of VICTORIA Input

```

1000.0 1000.0 1000.0 1000.0 1200.0 1200.0 1400.0 1700.0
1700.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1100.0 1100.0 1300.0 1600.0
1600.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1200.0 1500.0
1500.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1100.0 1400.0
1400.0 750.0 750.0 750.0 750.0 750.0 750.0

```

The format for gas temperature data, T_g , (K) is the same as for the fuel temperature data described in the preceding subsection.

\$ time values (s) for surface temperatures

```

0.    50.    150.    200.    250.    300.    350.    400.
900.  1000.  1050.  1100.  1150.  1200.  1250.

```

Following the gas temperature data is a set of time values (s) for structure surface temperatures. The values of time do not have to be the same as those given above; however, the same number of values must be given.

\$ ceiling temperatures (K)

```

1000.0 1500.0 1500.0 1500.0 1800.0 1800.0 2000.0 2300.0
2300.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1400.0 1400.0 1400.0 1700.0 1700.0 1900.0 2200.0
2200.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1300.0 1300.0 1300.0 1600.0 1600.0 1800.0 2100.0
2100.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1200.0 1200.0 1200.0 1500.0 1500.0 1700.0 2000.0
2000.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1100.0 1100.0 1100.0 1400.0 1400.0 1600.0 1900.0
1900.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1300.0 1300.0 1500.0 1800.0
1800.0 750.0 750.0 750.0 750.0 750.0 750.0

```

\$

```

1000.0 1000.0 1000.0 1000.0 1300.0 1300.0 1500.0 1800.0
1800.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1200.0 1200.0 1400.0 1700.0
1700.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1100.0 1100.0 1300.0 1600.0
1600.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1200.0 1500.0
1500.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1100.0 1400.0
1400.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1300.0
1300.0 750.0 750.0 750.0 750.0 750.0 750.0

```

\$

\$ wall temperatures (K)

```

1000.0 1500.0 1500.0 1500.0 1800.0 1800.0 2000.0 2300.0
2300.0 750.0 750.0 750.0 750.0 750.0 750.0

```

Description of VICTORIA Input

1000.0	1400.0	1400.0	1400.0	1700.0	1700.0	1900.0	2200.0
2200.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1300.0	1300.0	1300.0	1600.0	1600.0	1800.0	2100.0
2100.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1200.0	1200.0	1200.0	1500.0	1500.0	1700.0	2000.0
2000.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1100.0	1100.0	1100.0	1400.0	1400.0	1600.0	1900.0
1900.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1000.0	1000.0	1000.0	1300.0	1300.0	1500.0	1800.0
1800.0	750.0	750.0	750.0	750.0	750.0	750.0	
\$							
1000.0	1000.0	1000.0	1000.0	1300.0	1300.0	1500.0	1800.0
1800.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1000.0	1000.0	1000.0	1200.0	1200.0	1400.0	1700.0
1700.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1000.0	1000.0	1000.0	1100.0	1100.0	1300.0	1600.0
1600.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1200.0	1500.0
1500.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1100.0	1400.0
1400.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1300.0
1300.0	750.0	750.0	750.0	750.0	750.0	750.0	
\$							
\$ floor temperatures (K)							
1000.0	1500.0	1500.0	1500.0	1800.0	1800.0	2000.0	2300.0
2300.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1400.0	1400.0	1400.0	1700.0	1700.0	1900.0	2200.0
2200.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1300.0	1300.0	1300.0	1600.0	1600.0	1800.0	2100.0
2100.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1200.0	1200.0	1200.0	1500.0	1500.0	1700.0	2000.0
2000.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1100.0	1100.0	1100.0	1400.0	1400.0	1600.0	1900.0
1900.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1000.0	1000.0	1000.0	1300.0	1300.0	1500.0	1800.0
1800.0	750.0	750.0	750.0	750.0	750.0	750.0	
\$							
1000.0	1000.0	1000.0	1000.0	1300.0	1300.0	1500.0	1800.0
1800.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1000.0	1000.0	1000.0	1200.0	1200.0	1400.0	1700.0
1700.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1000.0	1000.0	1000.0	1100.0	1100.0	1300.0	1600.0
1600.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1200.0	1500.0
1500.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1100.0	1400.0
1400.0	750.0	750.0	750.0	750.0	750.0	750.0	
1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1300.0
1300.0	750.0	750.0	750.0	750.0	750.0	750.0	

Description of VICTORIA Input

Corresponding to the time values for surface temperatures, given above, are the surface temperature (K) data for ceilings (T_c), walls (T_w), and floors (T_f). These data are given in the same order as the other transient thermal-hydraulic data described above.

\$ time values (s) for gas pressures

0.	50.	150.	200.	250.	300.	350.	400.
900.	1000.	1050.	1100.	1150.	1200.	1250.	

Following the surface temperature data are the time values (s) for total gas pressures (Pa). Again, these time values can be different than those given above; however, the same number of values must be given.

\$ gas pressures (Pa)

[illegible]

\$

[illegible]

Gas pressure, P , data are given in the same order as the other transient thermal-hydraulic data described above.

\$ time values (s) for bulk gas velocities

0.	50.	150.	200.	250.	300.	350.	400.
900.	1000.	1050.	1100.	1150.	1200.	1250.	

Following the gas pressure data is a set of time values (s) that corresponds to the bulk gas velocity data given below.

Description of VICTORIA Input

\$ radial bulk gas velocities

0.177702	0.282288	0.282288	0.056993	0.067043	0.067366	0.074525
0.084992	0.080954	0.026464	0.026464	0.132322	1.058578	1.058578
1.058578						
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000						
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000						
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000						
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000						
-0.178345	-0.176430	-0.176430	-0.040507	-0.035286	-0.040576	-0.045732
-0.052924	-0.025409	-0.026464	-0.026464	-0.132322	-1.058578	-1.058578
-1.058578						

\$

0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000						
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000						
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000						
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000						
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000						
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000						

\$

\$ axial bulk gas velocities

0.261902	0.416044	0.416044	0.083998	0.098810	0.099287	0.109837
0.125263	0.119313	0.039004	0.039004	0.195020	1.560163	1.560163
1.560163						
0.265236	0.390041	0.390041	0.080415	0.093610	0.095061	0.105911
0.120944	0.104007	0.039004	0.039004	0.195020	1.560163	1.560163
1.560163						
0.259943	0.352853	0.352853	0.074513	0.085693	0.088074	0.098887
0.113031	0.086762	0.037806	0.037806	0.189028	1.512226	1.512226
1.512226						
0.262251	0.327649	0.327649	0.071065	0.080652	0.084004	0.095111
0.108793	0.073818	0.037806	0.037806	0.189028	1.512226	1.512226

Description of VICTORIA Input

```

1.512226
0.263918 0.302445 0.302445 0.067599 0.075611 0.079930 0.091327
0.104512 0.061970 0.037806 0.037806 0.189028 1.512226 1.512226
1.512226
2.078671 2.218219 2.218219 0.511109 0.564638 0.628087 0.730330
0.811274 0.401918 0.302484 0.302484 1.512422 12.099377 12.099377
12.099377
$
0.252234 0.274478 0.274478 0.057559 0.069867 0.071454 0.081884
0.096062 0.082974 0.037429 0.037429 0.187144 1.497151 1.497151
1.497151
0.252234 0.249525 0.249525 0.054635 0.064877 0.067683 0.078433
0.091906 0.071606 0.037429 0.037429 0.187144 1.497151 1.497151
1.497151
0.244787 0.242159 0.242159 0.054688 0.058118 0.062061 0.072808
0.085137 0.059298 0.036324 0.036324 0.181619 1.452952 1.452952
1.452952
0.244787 0.242159 0.242159 0.055597 0.053275 0.058428 0.069482
0.081029 0.050144 0.036324 0.036324 0.181619 1.452952 1.452952
1.452952
0.244787 0.242159 0.242159 0.055597 0.048432 0.054783 0.066137
0.076865 0.042010 0.036324 0.036324 0.181619 1.452952 1.452952
1.452952
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000

```

Radial velocity, u , data (m/s) are given first, followed by axial data, v . These data are given in the same order as the other transient thermal-hydraulic data described above. While the default is for flow rate data to be prescribed as velocities, two other options are available. These are described in Subsection 6.5.5.

6.5.4 Mass Source Data

The mass source data section can be omitted unless aerosol or vapor sources need to be included in a calculation. Such data are included in nearly all VICTORIA calculations, with the exceptions of restart and subdomain coupling calculations, which are described in subsequent subsections.

```
**TDEPSRCE
```

The above line is the descriptor for this section of input and must be the first line of the section.

```
$ number of aerosol sources
1
```

The second line of this section input section specifies the number of aerosol sources.

Description of VICTORIA Input

```
$ number of time values
15
```

This parameter defines the number of time values that are expected in the following sets of data.

```
$ time values
0.    50.    150.    200.    250.    300.    350.    400.
900.  1000.  1050.  1100.  1150.  1200.  1250.
```

The time values (s) corresponding to the source rate data are defined on these lines. The following data must be included for each aerosol source. No more than one aerosol source can be defined for each node.

```
$ number of species in aerosol source
2
```

This parameter defines the number of condensed-phase species in the aerosol source.

```
$ aerosol    mass fraction
'CsIc'       0.5
'CsOHc'      0.5
```

Next, the species and their mass fractions (dimensionless) are defined. In this case the aerosol is composed of an equal mixture (by mass) of cesium iodide and cesium hydroxide.

```
$ node for aerosol source
$ axial level  radial ring
1              1
```

The location of the aerosol source in this example is specified to be the node $j = 1, i = 1$.

```
$ aerosol source rates (kg/s)
15*0.001
```

These data tabulate the aerosol source rates (kg/s) for each time value given above. In this case, the aerosol source rate is a uniform rate of 1 g/s.

```
$ sigma    mass median radius (m)
2.00       0.5e-7
```

The final input data for an aerosol source define the size distribution of the aerosol. The distribution, by assumption, is log normal. It is specified by a standard deviation (dimensionless) and mass median radius (m). These terms are defined in Section 5.8.

Following the aerosol source data are the vapor source data.

Description of VICTORIA Input

```
$ number of vapor sources
2
```

In this example, there are two vapor sources. These sources are specified by the following set of parameters.

```
$ number of time values for vapor arrays
15
```

This parameter determines the number of time values that are expected in the following sets of data.

```
$ time values
    0.    50.   150.   200.   250.   300.   350.   400.
  900.  1000.  1050.  1100.  1150.  1200.  1250.
```

The time values (s) corresponding to the source rate data are defined on these lines. Following this, the source rate data are specified.

```
$ species name  axial level  radial ring
'H2Og'         1            1
$
$ source rates (kg/s)
  2.52    2.52    2.52    0.504    0.504    0.504    0.252    0.252
  0.0252  0.0252  0.0252  0.126    1.008    2.016    2.016
```

The first parameter specifies the species for the vapor source, which in this example is steam. The subsequent two parameters specify the node for which the source is defined. The last two lines of data define the mass source rate (kg/s) of steam for this node at each time value listed in the table above.

```
$ species name  axial level  radial ring
'H2g'          1            1
$
$ source rates (kg/s)
  0.0     0.0     0.0     0.0     0.0     0.0     0.028    0.028
  0.0028  0.0028  0.0028  0.014    0.112    0.0     0.0
```

The second mass source is defined using the same format as the first. In this example, the second mass source is for hydrogen. As indicated in this example, multiple vapor sources can be specified in a node.

6.5.5 Namelist Parameters

Subsection 6.3.8 describes the namelist parameters that are connected with static data; this subsection describes those that are connected with transient data. These namelist parameters cannot be interchanged, i.e., namelist parameters must be modified in the appropriate block of input data, either static or transient.

Description of VICTORIA Input

The namelist section of input data is not normally included in a VICTORIA calculation. It is provided as a means of gaining access to variables that are not normally modified.

```
**NAMELIST
```

The above line is the descriptor for this section of input and must be the first line of the section. The syntax required to modify a namelist parameter in the transient block of data is as follows:

```
$nametr
  betaf1 = 1.0
  betagp = 1.0
  betaml = 1.0
  betamn = 0.0001
  betafr = 0.001
  eta    = 0.0
  iaero  = (set in initialization data described in Section 6.2)
  icptim = 0
  ionoff = 50*0
  isorp  = 0
  lbflag = 0
  maxcls = 60
  tfroth = 2300.
  thresh = 1.0e12
  vblthk = 0.0
  zeta   = 0.5
  lvunit = 0
  lvzcal = 0
$end
```

Note that the dollar signs must be indented one space to distinguish these lines from comments. The values given above are the defaults that would be obtained if this section of input were omitted. Only those namelist parameters that are to be modified from the default value need be included in this section of data; those that are not included will retain their default values. The above variables have the following meanings:

- betaf1 Interconnected porosity (dimensionless) of the cladding (β_{fail} in Subsection 2.1.4) when it exceeds the prescribed failure temperature. The default value was the same in previous versions of VICTORIA.
- betagp Interconnected porosity (dimensionless) of the gap (β_z in Subsection 2.1.3). The default value was the same in previous versions of VICTORIA.
- betaml Interconnected porosity (dimensionless) of the cladding (β_{melt} in Subsection 2.1.4) when it exceeds the prescribed melting temperature. The default value was the same in previous versions of VICTORIA.
- betamn Initial interconnected porosity (dimensionless) of the fuel (β_0 in Subsection 2.1.2). The default value was the same in previous versions of VICTORIA.

Description of VICTORIA Input

betafr	Interconnected porosity (dimensionless) of the fuel (β_{fr} in Subsection 2.1.2) when frothing conditions are satisfied. The default for this parameter was 0.35 in previous versions of VICTORIA.
eta	Numerical tolerance used in calculating zeros of a function. The default value was the same in previous versions of VICTORIA.
iaero	Aerosol flag that is first set in the initialization block of input, as described in Section 6.2. At the start of each computation initiated by a COMPUTE command (described below), aerosol modeling is governed by this flag. The options for this flag are: 0 no aerosol modeling is performed 1 aerosol behavior is modeled, resuspension triggering is reset 2 aerosol behavior is modeled, but resuspension is inactive
icptim	If this flag is greater than 0, information is printed to the output file (discussed in Chapter 7) at each time step.
ionoff	An array of flags that are intended to be used only for code development purposes.
isorp	A flag that activates the optional chemisorption models described in Subsection 4.2.2. The default value was the same in previous versions of VICTORIA.
lbflag	A flag that controls whether a Nusselt number correlation is used to determine thermal boundary layer thickness. When this flag is 0, the correlation is used; otherwise, the thermal boundary layer thickness has a fixed value that is determined by the parameter vblthk.
maxcls	A parameter that determines the maximum number of attempts to calculate the zero of a function. The default value was the same in previous versions of VICTORIA.
tfroth	The temperature (K) at which fuel frothing occurs under reducing conditions (T_{fr} in Subsection 2.1.2). The default for this parameter was 2200 K in previous versions of VICTORIA.
thresh	Parameter representing a threshold in aerosol number density ($1/m^3$) below which heterogeneous nucleation is triggered, as described in Section 5.4. The default value was the same in previous versions of VICTORIA.
vblthk	Thermal boundary layer thickness (m). When lbflag is 0, this parameter is calculated from a Nusselt number correlation, as described in Subsection 5.6.4. When lbflag is not 0, this parameter has a constant value that can be set by the user. The default value was the same in previous versions of VICTORIA.
zeta	Numerical tolerance used in calculating zeros of a function. The default value was the same in previous versions of VICTORIA.
lvunit	Flag used to specify the units used for flow rates. The possible options are 0 flow rates are specified as velocities (m/s) 1 flow rates are specified as equivalent mass rates of steam (kg/s) 2 flow rates are specified as molar rates (kg-mol/s)
lvzcal	Flag that specifies how axial velocities are calculated. Possible values are

Description of VICTORIA Input

- 0 axial velocities are calculated from data in the input file, as described in Subsection 6.5.3.
- 1 axial velocities are computed assuming that mass sources into the bottom node of a ring correspond to mass flows upward through the domain. Radial flows are assumed to be zero. Axial velocity data in the input file are ignored.
- 2 axial velocities are computed assuming that mass sources into the bottom node of a ring correspond to mass flows upward through the domain. Radial flows are assumed to be zero. Axial velocity data omitted in the input file.

When `lvunit` is 1, mass flow rates are converted to molar flow rates assuming that the molecular weight of the gas is that of steam. The reason is that, in many cases, some of the steam is reduced to hydrogen. When this occurs, molar flow rates are conserved but mass flow rates are not. Option 2 is more versatile than option 1 and should generally be used when steam (which may be converted to hydrogen oxidation processes) is not the sole carrier gas.

6.5.6 Subdomain Coupling Data

Subdomain coupling is a new feature in VICTORIA 2.0. The concept is to allow a domain to be divided into two or more subdomains. Subdomain coupling is done by saving mass rate data that exit one subdomain on a file; these data are then read to specify mass sources for another subdomain. Both vapor and aerosol data are stored in the file.

Subdomain coupling can be done in order to facilitate sensitivity studies or to nodalize an irregular domain in ways that could not be done in any other way, given the limitations of the VICTORIA nodalization procedure. Some of these advantages are made more apparent in the following discussion. One limitation of subdomain coupling is that the flows between subdomains must be unidirectional; circular or return flows are not allowed. The guiding principle is that the subdomains must be able to be analyzed sequentially in order for this technique to work.

This section of input data is optional and is normally included in an input file only when subdomain coupling is being used.

****TDEPCOUP**

The above line is the descriptor for this section of input and must be the first line of the section.

\$ read (y=1;n=0)	write	write frequency	radial boundary
0	1	100	0

Description of VICTORIA Input

The next line contains four parameters. The first of these indicates whether a subdomain coupling file is to be read and is used to provide mass source input for the current calculation. The second parameter indicates whether a subdomain coupling file is to be written during the current calculation. The third parameter specifies a write frequency, in terms of the number of time steps. In this example, data are written to the file every 100 time steps. The final parameter on this line specifies whether data are to be written at a node on the radial boundary. The options for this parameter are the following:

- 0 data are written for flow exiting all nodes along the upper axial boundary.
- > 0 in addition to the nodes along the upper axial boundary, data are written for flow exiting one node on the outer radial boundary. The value of j corresponding to this node is specified by the value of this parameter.

The subdomain coupling technique can be used even when the number of radial rings in the two subdomains are not identical. For example, when the subdomain for the first calculation has more rings than the subdomain for the subsequent calculation, the data are summed and used as a mass source for the innermost ring; when the subdomain for the first calculation has fewer rings than the subdomain for the subsequent calculation, the data for each ring of the first calculation are used to provide a mass source for the same ring of the second calculation. These two situations are illustrated in Figure 6.2.

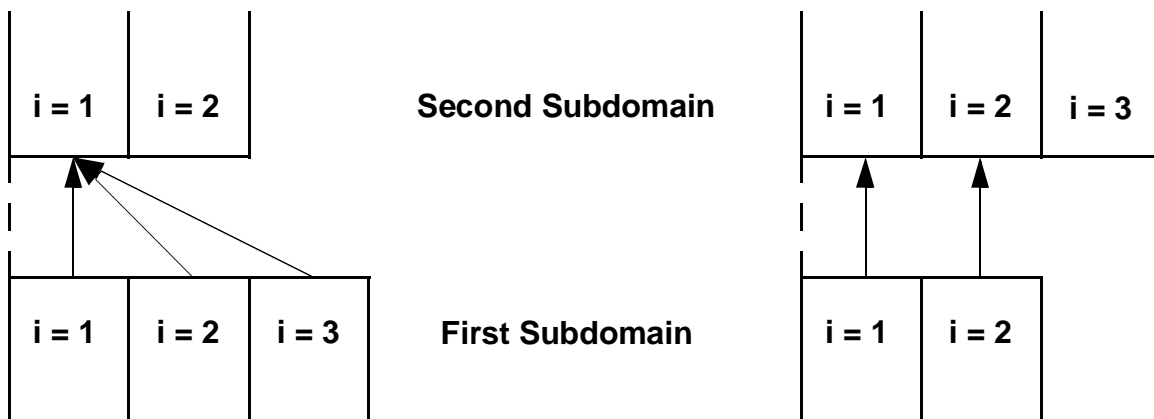


Figure 6.2. Illustration of mass flows between nodes when subdomains have different numbers of rings.

The concepts illustrated in Figure 6.2 can be quite useful for nodalizing irregular domains where it is advantageous to use a different number of rings in one subdomain than in another. The situation that is most likely to be useful is when the first subdomain is nodal-

Description of VICTORIA Input

ized with two or more rings and the second subdomain, possibly representing a circuit, is nodalized with a single ring. This situation is accommodated in a natural way by the subdomain coupling technique.

```
$ file to be read    file to be written
  'test.dum'        'test.bdy1'
```

The final line of data provides the names of the data files to be read and written. In this example no data file is to be read, so the name that is specified is a dummy that is never used. The naming conventions for subdomain coupling files to be written are to append a `.z` if the data correspond to the axial boundary and to append a `.r` if the data correspond to a radial boundary. In this example, since no data at a radial boundary are requested to be written, a single file named `test.bdy1.z` is created. This file name, including the `.z` extension, must be specified as the subdomain coupling “file to be read” in the input file for the second subdomain.

6.5.7 Time-Step and Output Data

This section of input controls time stepping and the frequency that output data are written. This section of data is required in all VICTORIA calculations.

```
**TDEPCTRL
```

The above line is the descriptor for this section of input and must be the first line of the section.

```
$  start time ; time step ; end time
    0.0         1.0         1100.0
```

The second line contains three parameters. The first is the initial time (s) for the VICTORIA calculation. The second parameter is the time-step size (s), which in this example is 1 s. Most commonly, time-step size is in the range of 0.001 s to 1 s. Constraints on time-step size are the Courant limit and the time scale for gas-phase diffusion, which are described in Chapter 7. The final parameter on this line is the end time (s) of the calculation.

```
$ print frequency    graphics frequency    output    write restart file
    1100              100                   0        1
```

The next line of input specifies the frequency (dimensionless) with which data are printed to the output and graphics files, in terms of the number of time steps, a flag to limit the data in the output file, and a flag to determine whether a restart file will be written. In this example, data are written to the output file every 1100 time steps and to the graphics file every 100 time steps. These files are described in Chapter 7. Options for the output flag are as follows:

Description of VICTORIA Input

- 0 full output
- 1 full output
- 2 output includes only aerosol data
- 3 output includes only chemistry data
- 4 abbreviated output--temperatures, pressures, and element mass data are not included

It is often wise, especially for long runs, to write restart files. This option provides a safeguard in case of a power failure or computer crash. When this option is selected, data are automatically written to the restart file every 30 minutes of CPU time. Data written to a restart file are not appended; rather, they overwrite previous data. Thus, a restart file contains only the last data that were written to it. Multiple restart files can be created by including multiple TDEPCTRL and COMPUTE sections in an input file, as explained below. Input files for restart runs are described in Section 6.7.

```
'test.rst1'
```

The final line of data in this section is the name of the restart file to be created. This line should be included only when a restart file is being written, as specified by the restart flag.

6.5.8 Initiation of Calculation

This section of input data consists of a single command, which instructs the code to begin a calculation. The calculation will normally continue until the final time specified in the TDEPCTRL section of input is reached, unless an error is encountered or a computer crash occurs. Processing of errors and error messages is discussed in Chapter 7.

```
**COMPUTE
```

More than one COMPUTE command can be issued in a single VICTORIA run. Generally, it is necessary to include the TDEPCTRL section of input between COMPUTE commands in order to redefine the end time of the calculation. Time-step size and other parameters, such as the name of the restart file being created, may be redefined as well. The initial time on the second line of the TDEPCTRL input section should be left blank by inserting a comma, because the start time is defined by the end time of the previous computation. Thus, for all but the first occurrence of the TDEPCTRL section of input, the second line of data should have the following format:

```
$  start time ; time step ; end time  
    , 0.1          1250.0
```

Description of VICTORIA Input

Parameters defined in each of the sections of input in the transient block of input data remain in effect unless they are modified. If the user wishes to modify any of the previously defined parameters, then any or all of the sections of input in the transient block of input data can be included between COMPUTE commands.

6.5.9 Data Not Used in the Current Calculation

For convenience, a section in the transient block of input data can be temporarily deactivated by replacing the descriptor with the following line:

```
**NOTUSED
```

When this descriptor appears in the input file, the input reader will search for the next descriptor and continue reading from there. In most cases, it is convenient to comment out the original descriptor rather than actually removing it. The NOTUSED descriptor must appear after the end of another section of input data; it cannot appear in the middle of a section of input data.

6.6 End of Calculation

The termination of a VICTORIA run is designated by the following command:

```
**END
```

This command does not need to be the final line of an input file; lines of input data following the END command are ignored and not executed.

6.7 Restart Runs

Calculations can be restarted if a restart file has been saved, as discussed in Subsection 6.5.7. The input file for a restart run is very much abbreviated from what is described above because nearly all of the input data from the run creating the restart file are contained on the restart file; thus, these input data do not need to be repeated in the input for the restart run. A sample restart input file is included below.

```
$ Computer type
  'Sparc 20'
$ Calculation Description
  'Restart of Test Problem (NEB)'
```

The first two lines of input contain computer and calculation descriptions, as described in Section 6.2.

```
$ restart
$ -----
  1
```


Description of VICTORIA Input

The second line of input indicates that this is a restart run.

```
$ file name for restart
test.rst1
```

The third line of input provides the name of the restart file that will be read.

```
**NAMELIST
$nametr
tfroth = 2350.
$end
```

Optionally, any of the sections in the transient block of input can be included, just as they can between two COMPUTE commands. In this example, the NAMELIST section is used to redefine the fuel frothing temperature.

```
**TDEPCOUP
$ read (y=1;n=0)   write   write frequency   outflow boundary
0                 1       100                0
$ file to be read   file to be written
'test.dum'          'test.bdy2'
```

The variables contained in the subdomain coupling section of the original input file are not saved in the restart file; thus, if this section of input was included in the original input file, it must also be included in the restart file. The name of the file to be written is different here than it was in the original TDEPCOUP section of input. This is essential; otherwise, the original file will be overwritten and the data from the original run will be lost.

When two (or more) subdomain coupling files are created, as would be the case when a restart is performed, the subsequent calculation that reads the subdomain coupling data must be performed with two (or more) COMPUTE commands. The first command (or set of commands) should perform calculations up to the point of restart and should read from the first subdomain coupling file. Following the first COMPUTE command should be a second TDEPCOUP input section, redefining the name of the subdomain coupling file to be read. Then the second COMPUTE command continues execution from the point of restart, reading data from the second subdomain coupling file.

```
**TDEPCTRL
$ start time ; time step ; end time
, 1.0         1200.0
$ print frequency   graphics frequency   output   write restart file
1100               100                   0        1
$ restart file name
'test.rst2'
```

Description of VICTORIA Input

Although it is not essential to include a TDEPCTRL section of input in a restart file, it is usually a good idea to do so. The start time must be left blank because the calculation will be started from the time that is read from the restart file. Other parameters can be redefined. In this example, the end time has been extended and the restart file name has been modified so that original restart file (the one that is used to perform the current restart) will not be overwritten.

```
**COMPUTE
```

The restart file must contain one or more COMPUTE commands.

```
**END
```

Computations are terminated by an END command, just as in a normal input file.

6.8 Running VICTORIA

There are two ways to run the VICTORIA code. The first way, which is the simpler of the two, is to use a script. The second is to enter all of the arguments on a UNIX command line. The syntax to initiate the script is as follows:

```
run v2.0 test
```

The script called `run` must be in the user's path and the user must have execute permission. Likewise, the VICTORIA executable, `v2.0`, must be in the user's path. If either `run` or `v2.0` is not in the user's path, an absolute or relative pathname can be substituted on the command line. For example,

```
./run ./v2.0 test
```

will work, provided that `run`, `v2.0`, and `test.inp` are all local files and that the user has execute permission for `run` and `v2.0`. The `run` script automatically appends `.inp` to the third argument, so the input file for this run should be named `test.inp`.

The `run` script will generate four files, which are described in Chapter 7. These files are assigned the following names:

```
test.gPID  
test.mPID  
test.oPID  
test.tPID
```

Each of the names of the four generated files begins with the name of the input file, truncated after the period. In other words, the `inp` designating the input file is omitted. The letter following the period designates the type of file: `g` designates a binary graphics file; `m` designates a message file which may contain error messages at the operating system

Description of VICTORIA Input

level; `o` designates an ascii-formatted output file; and `t` designates a progress file that contains information on each time step. The final portion of the name is the process ID, which ensures that the generated file names will be unique. Each of these files is described in Chapter 7.

The second way to run VICTORIA is to enter the command initiating execution manually, as follows:

```
v2.0 test.inp test.out test.tty test.grf
```

Using this command, the user is responsible for naming each of the files. Some caution should be exercised when making multiple simultaneous runs that the generated files do not conflict. Using the above syntax will cause error messages at the operating system level to be written directly to the window or terminal screen from which the command line was entered. Alternatively, error output can be redirected to a file named `test.msg` by using the following command syntax in a C shell:

```
v2.0 test.inp test.out test.tty test.grf >& test.msg
```

or the following syntax in a Bourne shell:

```
v2.0 test.inp test.out test.tty test.grf 2> test.msg
```

Description of VICTORIA Input

7.0 Description of VICTORIA Output

Running VICTORIA via the `run` script generates four output files. These same files can also be generated by entering the requisite file names manually on a command line. Both procedures are described in Section 6.8. This chapter describes each of the generated files. Section 7.1 describes the output file, which is a readable file in ASCII format. Section 7.2 describes the progress file, which contains a brief description of each time step and is also in ASCII format. Section 7.3 describes the graphics file, which is in binary format. Finally, Section 7.4 describes a message file, which contains error messages at the operating system level.

7.1 Output File

The output file contains a number of sections of information, which are illustrated for the input file described in Chapter 6. The first of these contains basic information on the run, computer, and files used in the run. This section of output is described in Subsection 7.1.1. The second section is a direct echo of the input file, which is useful for identification of the input parameters that were used for the run. This section of output is described in Subsection 7.1.2. The third section in the output file is an interpreted description of the input, which is useful for spotting errors. This section of output is described in Subsection 7.1.3. The next nine sections of output contain information about the solution after the first time step and other time steps where output is requested by the user. The frequency of this output is controlled by a parameter in the input file, as described in Subsection 6.5.7. These nine sections of output, which may be repeated a number of times in the output file, are described in Subsections 7.1.4 through 7.1.12. The final subsection, 7.1.13, describes error messages that can be generated and gives some guidance on how to modify the input to eliminate the errors.

7.1.1 Basic Information

The first section of output contains very basic information on the computer and files that were used to perform the run. At the top of this (and every) page of output are two lines that describe the VICTORIA version number, with creation date, and the current date and time when the page was written.

```
1
1998
1998 page 1
VICTORIA INPUT DATA
Job Details
Process ID      pid18375
User            nbixler
Hostname        SunOS sun4m      homeboy
Working Directory /u7/nbixler/victoria/v1.x/viki/test
Executable ls -l lrwxrwxrwx 1 nbixler      7 Feb 12 16:41 v2.0 -> ../v2.0
Input deck ls -l -rw-rw-rw- 1 nbixler    21853 Mar  3 14:44 i3.inp
Date & Time     Tue Mar  3 14:44:58 MST 1998
Victoria 2.0 1 Jul
Tue Mar  3 21:44:58
```

Description of VICTORIA Output

The subsequent lines give the process identification number, the user name, the host name and type of operating system, the directory in which the run was performed, the executable name, the input file name, and the date and time when the run was initiated. This information is sometimes useful when multiple runs are performed with variations of an input file or with different versions of VICTORIA.

7.1.2 Echo of Input

The second section of the output file contains a direct echo of the input file. This information is often useful for identifying the exact input file that was used with a calculation, especially when sensitivity studies are being performed.

```
$
$ *****
$           Input deck for VICTORIA 2.0
$ *****
$
$ Test deck to put the code through its paces
$
$ Job details
$ -----
$ Computer type:
$ 'Sparc 20'
$ Calculation Description:
$ 'Test Problem (NEB)'
$
$   restart
$   -----
$   0
$
$           internal sub-module selection
$ -----
$ chemistry  aerosols  advection  release  decay oxidation
$    2         2         1         1         1         1
$
$           Geometrical Data
$           -----
$ axial ; radial ; fuel radial ; clad radial
$    6      2      2      1
$
$ general cell input section
$ -----
$   central radii
$   6*0.0
$
$ radial widths
$   6*0.7
$   6*0.3
$ axial heights
$   6*0.5
$
$
$ **FUELDATA
1
1998
1998 page      2
1998          VICTORIA INPUT DATA
1998          2

$ pellet diam. ; gap thick. ; clad thick. ; Helium pressure ; frac. theo. dens
$ 8.2E-03      1.6E-04      6.0E-04      2.5E+06      0.96
$ initial clad oxide level
$ 0.0
$ number of fuel rods per node
$ 2*5, 4*0
$ 2*5, 4*0
$
$ permeabilities
$ fuel      gap radial  gap axial  cladding radial  film radial
Victoria 2.0  1 Jul
Tue Mar  3 21:44:59
```

Description of VICTORIA Output

```

1.e-15  1.e-13      1.e-13      1.e-14      1.e-13
$
$ Number of Elements in the Fuel grains
15
$
$ Fuel grain inventories and diffusion coefficients
$
  'U'
$ dzero ; theta
    37.79  ' 37.79  '
    37.79  37.79
    37.79  37.79
    37.79  37.79
$
  'O'
$ dzero ; theta
    76.3358  ' 76.3358  '
    76.3358  76.3358
    76.3358  76.3358
    76.3358  76.3358
$
  'Cs'
$ dzero ; theta
    0.118  ' 0.118  '
    0.118  0.118
    0.118  0.118
    0.118  0.118
$
  'Ba'
$ dzero ; theta
    6.311e-2  ' 6.311e-2  '
    6.311e-2  6.311e-2
    6.311e-2  6.311e-2
    6.311e-2  6.311e-2
$
  'I'
$ dzero ; theta
1
1998
      VICTORIA  INPUT  DATA
1998 page      3

    0.0091  ' 0.0091  '
    0.0091  0.0091
    0.0091  0.0091
    0.0091  0.0091
$
  'Sr'
$ dzero ; theta
    0.064  ' 0.064  '
    0.064  0.064
    0.064  0.064
    0.064  0.064
$
  'Zr'
$ dzero ; theta
    0.228  ' 0.228  '
    0.228  0.228
    0.228  0.228
    0.228  0.228
$
  'Sn'
$ dzero ; theta
    0.0024  ' 0.0024  '
    0.0024  0.0024
    0.0024  0.0024
    0.0024  0.0024
$

```

Victoria 2.0 1 Jul
 Tue Mar 3 21:44:59

Description of VICTORIA Output

```

'Te'
$ dzero ; theta
    0.019 ' 0.019 '
    0.019 0.019
    0.019 0.019
    0.019 0.019
$
'Kr'
$ dzero ; theta
    0.026 ' 0.026 '
    0.026 0.026
    0.026 0.026
    0.026 0.026
$
'Xe'
$ dzero ; theta
    0.228 ' 0.228 '
    0.228 0.228
    0.228 0.228
1
1998 Victoria 2.0 1 Jul
1998 page 4 Tue Mar 3 21:44:59
    0.228 0.228
$
'Mo'
$ dzero ; theta
    0.188 ' 0.188 '
    0.188 0.188
    0.188 0.188
    0.188 0.188
$
'Ru'
$ dzero ; theta
    0.132 ' 0.132 '
    0.132 0.132
    0.132 0.132
    0.132 0.132
$
'Sb'
$ dzero ; theta
    0.0009 ' 0.0009 '
    0.0009 0.0009
    0.0009 0.0009
    0.0009 0.0009
$
'Eu'
$ dzero ; theta
    0.0057 ' 0.0057 '
    0.0057 0.0057
    0.0057 0.0057
    0.0057 0.0057
$
$ grain diameters
2*1.0e-5
2*1.0e-5
2*1.0e-5
2*1.0e-5
$
$
**CORODATA
$
$ absorber control rod cladding
$ diam. length int. diam. ext. diam. length
8.66e-3 0.90 8.7e-3 9.7e-3 1.00
$
$ mass fraction helium fill
$ Ag In Cd pressure (Pa)

```


Description of VICTORIA Output

```

0.80 0.15 0.05 1.5e5
$
$ number of control rods
1
1998
VICTORIA INPUT DATA
1998 page 5

2*1,4*0
2*1,4*0
$
$
**STRUADATA
$
$ Flags for inner rings
$ flow irregularity flags
3*0 3 4 2
$ node 4 steam separator information
$ tube length tube radius vane angle (rad)
0.05 0.15 0.52
$ node 5 steam dryer information
$ no. of bends tube angle (rad) bend spacing
5 1.04 1.5
$ node 6 abrupt contraction information
$ inlet diam. exit diam
0.7 0.35
$ Flags for outer rings
$ flow irregularity flags
1 2*0 3 4 1
$ node 4 steam separator information
$ tube length tube radius vane angle (rad)
0.05 0.15 0.52
$ node 5 steam dryer information
$ no. of bends tube angle (rad) bend spacing
5 1.04 1.5
$
$ settling parameters
6*-1.0
6*-1.0
$
$ axial flow areas
2*1.4921,3*1.5394,0.3848
2*1.5549,3*1.6022,0.0
$
$ radial flow areas
6*2.1991
6*0.0
$
$ hydraulic diameters
2*0.3630,4*1.4
2*0.2757,4*1.02
$
$ floor area in node
1.1545,5*0.0
1.6022,5*0.0
$
$ wall area in node
6*0.1
6*3.1416
$
1
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$ ceiling area in node
5*0.0,1.1545
5*0.0,1.6022
$
$ structure identification flags
6*0
1,2,3,4,5,6
$
$
**CONTDATA
$

```

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Description of VICTORIA Output

```

$ initial species present
1
$ species name
'H2Og'
$ species mass concentrations
6*3.2475
6*3.2475
$
$
**DECAY
$
$ decay heat initialization flag
2
$
$ insulation    time since    reactor power (kW)
$ temperature   scram
300.           0.           10.0
$
$ structure failure temperature
2500.
$
$ heatup flags at boundary
$ inner upper bottom outer
6*0    2*1    2*0    6*1
$
$ thicknesses of pipe walls (m)
16*0.005
$
$ thermal conductivity of the insulation (W/m/K)
16*0.001
$
$ thicknesses of the insulation (m)
16*0.05
$
$
**AERODATA
$
$ Definition of collocation points
$ ncoll    ;    spacing
,
,
$
1
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$ mlower ; mupper
,
,
$
$ element number
,
,
$
$ Tolerance specification
$ eps ; maxtrys
,
,
$
$ Aerosol physics data
$ cshpfctr dshpfctr stickeff
1.0 1.0 1.0
$ k1 k2 k3
1.25 0.41 0.88
$ cmbrock csbrock ctbrock
1.14 1.17 2.18
$
$
**PAUSE
$
$
**TDEPCHEM
$
$ Numerical Control data
$ -----
$ max chem. iter. ; convergence criterion ; max cyclic Newton iter.
200 1.e-8 20
$

```

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Description of VICTORIA Output

```

$
$ gas diff. (0,1,2); frozen chem on/off (1/0); temp threshold (K)
1 0 1000.
$
$
**TDEPFUEL
$
$ fuel temperature interpolation parameter
1.0
$
$ number of time values for temperature arrays
15
$
$ time values (s) for fuel temperatures
0. 50. 150. 200. 250. 300. 350. 400.
900. 1000. 1050. 1100. 1150. 1200. 1250.
$
$ fuel center-line temperatures (K)
1050.0 1750.0 1750.0 1750.0 2050.0 2050.0 2250.0 2550.0
2550.0 1050.0 1050.0 1050.0 1050.0 1050.0 1050.0
1050.0 1650.0 1650.0 1650.0 1950.0 1950.0 2150.0 2450.0
2450.0 1050.0 1050.0 1050.0 1050.0 1050.0 1050.0
1
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15*0.0
15*0.0
15*0.0
15*0.0
$
1050.0 1250.0 1250.0 1250.0 1550.0 1550.0 1750.0 2050.0
2050.0 1050.0 1050.0 1050.0 1050.0 1050.0 1050.0
1050.0 1150.0 1150.0 1150.0 1450.0 1450.0 1650.0 1950.0
1950.0 1050.0 1050.0 1050.0 1050.0 1050.0 1050.0
15*0.0
15*0.0
15*0.0
15*0.0
$
$ fuel surface temperatures (K)
1025.0 1725.0 1725.0 1725.0 2025.0 2025.0 2225.0 2525.0
2525.0 1025.0 1025.0 1025.0 1025.0 1025.0 1025.0
1025.0 1625.0 1625.0 1625.0 1925.0 1925.0 2125.0 2425.0
2425.0 1025.0 1025.0 1025.0 1025.0 1025.0 1025.0
15*0.0
15*0.0
15*0.0
15*0.0
$
1025.0 1225.0 1225.0 1225.0 1525.0 1525.0 1725.0 2025.0
2025.0 1025.0 1025.0 1025.0 1025.0 1025.0 1025.0
1025.0 1125.0 1125.0 1125.0 1425.0 1425.0 1625.0 1925.0
1925.0 1025.0 1025.0 1025.0 1025.0 1025.0 1025.0
15*0.0
15*0.0
15*0.0
15*0.0
$
$ Cladding temperatures (K)
1000.0 1700.0 1700.0 1700.0 2000.0 2000.0 2200.0 2500.0
2500.0 1000.0 1000.0 1000.0 1000.0 1000.0 1000.0
1000.0 1600.0 1600.0 1600.0 1900.0 1900.0 2100.0 2400.0
2400.0 1000.0 1000.0 1000.0 1000.0 1000.0 1000.0
15*0.0
15*0.0
15*0.0
15*0.0
$
1000.0 1200.0 1200.0 1200.0 1500.0 1500.0 1700.0 2000.0
2000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1000.0
1000.0 1100.0 1100.0 1100.0 1400.0 1400.0 1600.0 1900.0
1900.0 1000.0 1000.0 1000.0 1000.0 1000.0 1000.0
15*0.0
15*0.0

```

Description of VICTORIA Output

```
15*0.0
15*0.0
$
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$ cladding failure temperature (K)
2000.0
$
$ cladding interconnected porosity when fully oxidized
0.05
$
$ cladding melt temperature
2100.0
$
$
**TDEPSTRU
$
$ time values (s) for gas temperatures
0. 50. 150. 200. 250. 300. 350. 400.
900. 1000. 1050. 1100. 1150. 1200. 1250.
$
$ gas temperatures (K)
1000.0 1600.0 1600.0 1600.0 1900.0 1900.0 2100.0 2400.0
2400.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1500.0 1500.0 1500.0 1800.0 1800.0 2000.0 2300.0
2300.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1400.0 1400.0 1400.0 1700.0 1700.0 1900.0 2200.0
2200.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1300.0 1300.0 1300.0 1600.0 1600.0 1800.0 2100.0
2100.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1200.0 1200.0 1200.0 1500.0 1500.0 1700.0 2000.0
2000.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1100.0 1100.0 1100.0 1400.0 1400.0 1600.0 1900.0
1900.0 750.0 750.0 750.0 750.0 750.0 750.0
$
1000.0 1100.0 1100.0 1100.0 1400.0 1400.0 1600.0 1900.0
1900.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1300.0 1300.0 1500.0 1800.0
1800.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1200.0 1200.0 1400.0 1700.0
1700.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1100.0 1100.0 1300.0 1600.0
1600.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1200.0 1500.0
1500.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1100.0 1400.0
1400.0 750.0 750.0 750.0 750.0 750.0 750.0
$
$ time values (s) for surface temperatures
0. 50. 150. 200. 250. 300. 350. 400.
900. 1000. 1050. 1100. 1150. 1200. 1250.
$
$ ceiling temperatures (K)
1000.0 1500.0 1500.0 1500.0 1800.0 1800.0 2000.0 2300.0
2300.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1400.0 1400.0 1400.0 1700.0 1700.0 1900.0 2200.0
2200.0 750.0 750.0 750.0 750.0 750.0 750.0
1
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1000.0 1300.0 1300.0 1300.0 1600.0 1600.0 1800.0 2100.0
2100.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1200.0 1200.0 1200.0 1500.0 1500.0 1700.0 2000.0
2000.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1100.0 1100.0 1100.0 1400.0 1400.0 1600.0 1900.0
1900.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1300.0 1300.0 1500.0 1800.0
1800.0 750.0 750.0 750.0 750.0 750.0 750.0
$
1000.0 1000.0 1000.0 1000.0 1300.0 1300.0 1500.0 1800.0
1800.0 750.0 750.0 750.0 750.0 750.0 750.0
```

Description of VICTORIA Output

```

1000.0 1000.0 1000.0 1000.0 1200.0 1200.0 1400.0 1700.0
1700.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1100.0 1100.0 1300.0 1600.0
1600.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1200.0 1500.0
1500.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1100.0 1400.0
1400.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1300.0
1300.0 750.0 750.0 750.0 750.0 750.0 750.0
$
$ wall temperatures (K)
1000.0 1500.0 1500.0 1500.0 1800.0 1800.0 2000.0 2300.0
2300.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1400.0 1400.0 1400.0 1700.0 1700.0 1900.0 2200.0
2200.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1300.0 1300.0 1300.0 1600.0 1600.0 1800.0 2100.0
2100.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1200.0 1200.0 1200.0 1500.0 1500.0 1700.0 2000.0
2000.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1100.0 1100.0 1100.0 1400.0 1400.0 1600.0 1900.0
1900.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1300.0 1300.0 1500.0 1800.0
1800.0 750.0 750.0 750.0 750.0 750.0 750.0
$
1000.0 1000.0 1000.0 1000.0 1300.0 1300.0 1500.0 1800.0
1800.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1200.0 1200.0 1400.0 1700.0
1700.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1100.0 1100.0 1300.0 1600.0
1600.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1200.0 1500.0
1500.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1100.0 1400.0
1400.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1300.0
1300.0 750.0 750.0 750.0 750.0 750.0 750.0
$
$ floor temperatures (K)
1000.0 1500.0 1500.0 1500.0 1800.0 1800.0 2000.0 2300.0
2300.0 750.0 750.0 750.0 750.0 750.0 750.0
1
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1000.0 1400.0 1400.0 1400.0 1700.0 1700.0 1900.0 2200.0
2200.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1300.0 1300.0 1300.0 1600.0 1600.0 1800.0 2100.0
2100.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1200.0 1200.0 1200.0 1500.0 1500.0 1700.0 2000.0
2000.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1100.0 1100.0 1100.0 1400.0 1400.0 1600.0 1900.0
1900.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1300.0 1300.0 1500.0 1800.0
1800.0 750.0 750.0 750.0 750.0 750.0 750.0
$
1000.0 1000.0 1000.0 1000.0 1300.0 1300.0 1500.0 1800.0
1800.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1200.0 1200.0 1400.0 1700.0
1700.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1100.0 1100.0 1300.0 1600.0
1600.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1200.0 1500.0
1500.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1100.0 1400.0
1400.0 750.0 750.0 750.0 750.0 750.0 750.0
1000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1000.0 1300.0
1300.0 750.0 750.0 750.0 750.0 750.0 750.0
$
$ time values (s) for gas pressures
0. 50. 150. 200. 250. 300. 350. 400.
900. 1000. 1050. 1100. 1150. 1200. 1250.
$
$ gas pressures (Pa)
15.e5 15.e5 15.e5 15.e5 15.e5 15.e5 15.e5 15.e5

```

```

1          1.5e5    1.5e5    1.5e5    1.5e5    1.5e5    1.5e5    1.5e5
15.e5     15.e5     15.e5     15.e5     15.e5     15.e5     15.e5     15.e5
1.5e5      1.5e5      1.5e5      1.5e5      1.5e5      1.5e5      1.5e5
15.e5      15.e5      15.e5      15.e5      15.e5      15.e5      15.e5     15.e5
1.5e5      1.5e5      1.5e5      1.5e5      1.5e5      1.5e5      1.5e5
15.e5      15.e5      15.e5      15.e5      15.e5      15.e5      15.e5     15.e5
1.5e5      1.5e5      1.5e5      1.5e5      1.5e5      1.5e5      1.5e5
15.e5      15.e5      15.e5      15.e5      15.e5      15.e5      15.e5     15.e5
1.5e5      1.5e5      1.5e5      1.5e5      1.5e5      1.5e5      1.5e5
15.e5      15.e5      15.e5      15.e5      15.e5      15.e5      15.e5     15.e5
1.5e5      1.5e5      1.5e5      1.5e5      1.5e5      1.5e5      1.5e5
$         15.e5      15.e5      15.e5      15.e5      15.e5      15.e5      15.e5
15.e5      15.e5      15.e5      15.e5      15.e5      15.e5      15.e5
15.e5      15.e5      15.e5      15.e5      15.e5      15.e5      15.e5     15.e5
1.5e5      1.5e5      1.5e5      1.5e5      1.5e5      1.5e5      1.5e5
15.e5      15.e5      15.e5      15.e5      15.e5      15.e5      15.e5     15.e5
1.5e5      1.5e5      1.5e5      1.5e5      1.5e5      1.5e5      1.5e5
15.e5      15.e5      15.e5      15.e5      15.e5      15.e5      15.e5     15.e5
1.5e5      1.5e5      1.5e5      1.5e5      1.5e5      1.5e5      1.5e5
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       15.e5    15.e5    15.e5    15.e5    15.e5    15.e5    15.e5    15.e5
$      1.5e5    1.5e5    1.5e5    1.5e5    1.5e5    1.5e5    1.5e5
$ time values (s) for bulk gas velocities
   0.    50.    150.    200.    250.    300.    350.    400.
$  900.  1000.  1050.  1100.  1150.  1200.  1250.
$ radial bulk gas velocities
0.177702  0.282288  0.282288  0.056993  0.067043  0.067366  0.074525
0.084992  0.080954  0.026464  0.026464  0.132322  1.058578  1.058578
1.058578
0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
-0.178345 -0.176430 -0.176430 -0.040507 -0.035286 -0.040576 -0.045732
-0.052924 -0.025409 -0.026464 -0.026464 -0.132322 -1.058578 -1.058578
-1.058578
0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
0.000000
0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
$ axial bulk gas velocities
0.261902  0.416044  0.416044  0.083998  0.098810  0.099287  0.109837
0.125263  0.119313  0.039004  0.039004  0.195020  1.560163  1.560163
1.560163

```

Description of VICTORIA Output

```

0.265236 0.390041 0.390041 0.080415 0.093610 0.095061 0.105911
0.120944 0.104007 0.039004 0.039004 0.195020 1.560163 1.560163
1.560163
1
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0.259943 0.352853 0.352853 0.074513 0.085693 0.088074 0.098887
0.113031 0.086762 0.037806 0.037806 0.189028 1.512226 1.512226
1.512226
0.262251 0.327649 0.327649 0.071065 0.080652 0.084004 0.095111
0.108793 0.073818 0.037806 0.037806 0.189028 1.512226 1.512226
1.512226
0.263918 0.302445 0.302445 0.067599 0.075611 0.079930 0.091327
0.104512 0.061970 0.037806 0.037806 0.189028 1.512226 1.512226
1.512226
2.078671 2.218219 2.218219 0.511109 0.564638 0.628087 0.730330
0.811274 0.401918 0.302484 0.302484 1.512422 12.099377 12.099377
12.099377
0.252234 0.274478 0.274478 0.057559 0.069867 0.071454 0.081884
0.096062 0.082974 0.037429 0.037429 0.187144 1.497151 1.497151
1.497151
0.252234 0.249525 0.249525 0.054635 0.064877 0.067683 0.078433
0.091906 0.071606 0.037429 0.037429 0.187144 1.497151 1.497151
1.497151
0.244787 0.242159 0.242159 0.054688 0.058118 0.062061 0.072808
0.085137 0.059298 0.036324 0.036324 0.181619 1.452952 1.452952
1.452952
0.244787 0.242159 0.242159 0.055597 0.053275 0.058428 0.069482
0.081029 0.050144 0.036324 0.036324 0.181619 1.452952 1.452952
1.452952
0.244787 0.242159 0.242159 0.055597 0.048432 0.054783 0.066137
0.076865 0.042010 0.036324 0.036324 0.181619 1.452952 1.452952
1.452952
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000
$
$
**TDEPSRCE
$
$ number of aerosol sources
1
$
$ number of time values for aerosol sources
15
$
$ time values
0. 50. 150. 200. 250. 300. 350. 400.
900. 1000. 1050. 1100. 1150. 1200. 1250.
$
$ number of species in aerosol source
2
$
$ aerosol mass fraction
'CsIc' 0.5
'CsOHc' 0.5
$
$ node for aerosol source
1
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$ axial level radial ring
1 1
$
$ aerosol source rates (kg/s)
15*0.001
$
$ sigma mass median radius (m)
2.00 0.5e-7
$
$ number of vapor sources
2

```

Description of VICTORIA Output

```

$
$ number of time values for vapor sources
15
$
$ time values
0.    50.    150.    200.    250.    300.    350.    400.
900.  1000.  1050.  1100.  1150.  1200.  1250.
$
$ species name  axial level  radial ring
'H2Og'         1           1
$
$ source rates (kg/s)
2.52    2.52    2.52    0.504    0.504    0.504    0.252    0.252
0.0252  0.0252  0.0252  0.126    1.008    2.016    2.016
$
$ species name  axial level  radial ring
'H2g'          1           1
$
$ source rates (kg/s)
0.0     0.0     0.0     0.0     0.0     0.0     0.028    0.028
0.0028  0.0028  0.0028  0.014    0.112    0.0     0.0
$
$
**TDEPCTRL
$
$ time step control input
$ -----
$ start time ; time step ; end time
0.0         1.0         1100.0
$
$ Output control
$ -----
$ print frequency ; graphics frequency ; output ; write restart file
1100         25         0         1
$
$ 'test.rst'
$
$
**COMPUTE
$
$
1
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**TDEPCTRL
$
$ time step control input
$ -----
$ start time ; time step ; end time
,          0.1         1250.0
$
$ Output control
$ -----
$ print frequency ; graphics frequency ; output ; write restart file
1500         250         0         1
$
$ 'test.rst'
$
$
**COMPUTE
$
$
**END

```

Notice that this section can be cut from the output file and used, with minor editing, as a VICTORIA input file. This is sometimes useful in case an input file is accidentally deleted or heavily modified from the one used to perform an earlier run.

Description of VICTORIA Output

7.1.3 Interpreted Echo of Input

The next section of the output file contains an interpreted echo of the input file. This section is often useful for finding errors in the input file. For example, this section can be helpful for tracing an input parameter that was accidentally omitted.

```

1 1998 VICTORIA INPUT DATA Victoria 2.0 1 Jul
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0 ***** Machine and Job Details *****

Victoria 2.0 1 Jul 1998

Calculations Performed on Sparc 20

with 26 elements 288 species, of which 110 can be aerosols

Test Problem (NEB)
***** Read dump Flag *****

0 irststr = 0
***** Option Control Data *****

0 icheM = 2 iaero = 2 iconvc = 1 irodr = 1 idecay = 1 ioxful = 1
***** Cell Data *****

Number of axial levels = 6
Number of radial rings = 2
Number of fuel nodes = 2
Number of clad nodes = 1
0 ***** Cell Geometrical Data *****

Inner radius of cell annulus=
0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
0 ***** Cell Widths *****
Widths = Radial ring number = 1
Widths =
0.7000E+00 0.7000E+00 0.7000E+00 0.7000E+00 0.7000E+00 0.7000E+00
0 ***** Cell Widths *****
Widths = Radial ring number = 2
Widths =
0.3000E+00 0.3000E+00 0.3000E+00 0.3000E+00 0.3000E+00 0.3000E+00
0 ***** Cell Heights *****
Heights =
0.5000E+00 0.5000E+00 0.5000E+00 0.5000E+00 0.5000E+00 0.5000E+00
0 cell interfaces are:
0.0000 0.5000 1.0000 1.5000 2.0000 2.5000 3.0000

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**FUELDATA
0 ***** Fuel Data *****
Pellet diameter = 8.2000E-03
Gap thickness = 1.6000E-04
Clad thickness = 6.0000E-04
Initial helium pressure = 2.5000E+06
Theoretical density = 9.6000E-01
Fraction of clad oxidized= 0.0000E+00
Fuel rods per axial level=
5 5 0 0 0 5 5 0 0 0 0
0 ***** Fuel Permeability Data *****
fuel gap clad film
radial axial radial axial radial axial radial axial
0.100E-14 0.000E+00 0.100E-12 0.100E-12 0.100E-13 0.000E+00 0.100E-12 0.000E+00
0 ***** Fuel Rod Release Data *****
number of fission products in fuel grains= 15
0 Fuel Inventory Species Number = 72 Species Name = Uc

```

Description of VICTORIA Output

```
0      DZERO = 0.0000E+00 THETA = 0.4500E+05
0      Fission Product Concentration =
      3.7790E+01 3.7790E+01
      3.7790E+01 3.7790E+01
      3.7790E+01 3.7790E+01
      3.7790E+01 3.7790E+01
0      Fuel Inventory Species Number = 80 Species Name = Og
0      DZERO = 0.0000E+00 THETA = 0.4500E+05
0      Fission Product Concentration =
      7.6336E+01 7.6336E+01
      7.6336E+01 7.6336E+01
      7.6336E+01 7.6336E+01
      7.6336E+01 7.6336E+01
0      Fuel Inventory Species Number = 8 Species Name = Csc
0      DZERO = 0.5000E-04 THETA = 0.4500E+05
0      Fission Product Concentration =
      1.1800E-01 1.1800E-01
      1.1800E-01 1.1800E-01
      1.1800E-01 1.1800E-01
      1.1800E-01 1.1800E-01
1
1998 Victoria 2.0 1 Jul
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0      Fuel Inventory Species Number = 22 Species Name = Bac
0      DZERO = 0.5000E-04 THETA = 0.4500E+05
0      Fission Product Concentration =
      6.3110E-02 6.3110E-02
      6.3110E-02 6.3110E-02
      6.3110E-02 6.3110E-02
      6.3110E-02 6.3110E-02
0      Fuel Inventory Species Number = 27 Species Name = Ig
0      DZERO = 0.5000E-04 THETA = 0.4500E+05
0      Fission Product Concentration =
      9.1000E-03 9.1000E-03
      9.1000E-03 9.1000E-03
      9.1000E-03 9.1000E-03
      9.1000E-03 9.1000E-03
0      Fuel Inventory Species Number = 42 Species Name = Src
0      DZERO = 0.5000E-04 THETA = 0.4500E+05
0      Fission Product Concentration =
      6.4000E-02 6.4000E-02
      6.4000E-02 6.4000E-02
      6.4000E-02 6.4000E-02
      6.4000E-02 6.4000E-02
0      Fuel Inventory Species Number = 50 Species Name = Zrc
0      DZERO = 0.5000E-04 THETA = 0.4500E+05
0      Fission Product Concentration =
      2.2800E-01 2.2800E-01
      2.2800E-01 2.2800E-01
      2.2800E-01 2.2800E-01
      2.2800E-01 2.2800E-01
0      Fuel Inventory Species Number = 51 Species Name = Snc
0      DZERO = 0.5000E-04 THETA = 0.4500E+05
0      Fission Product Concentration =
      2.4000E-03 2.4000E-03
      2.4000E-03 2.4000E-03
      2.4000E-03 2.4000E-03
      2.4000E-03 2.4000E-03
0      Fuel Inventory Species Number = 63 Species Name = Tec
0      DZERO = 0.5000E-04 THETA = 0.4500E+05
0      Fission Product Concentration =
      1.9000E-02 1.9000E-02
      1.9000E-02 1.9000E-02
      1.9000E-02 1.9000E-02
      1.9000E-02 1.9000E-02
1
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0      Fuel Inventory Species Number = 77 Species Name = Krg
0      DZERO = 0.5000E-04 THETA = 0.4500E+05
0      Fission Product Concentration =
      2.6000E-02 2.6000E-02
```

Description of VICTORIA Output

```

2.6000E-02 2.6000E-02
2.6000E-02 2.6000E-02
2.6000E-02 2.6000E-02
0 Fuel Inventory Species Number = 78 Species Name = Xeg
0 DZERO = 0.5000E-04 THETA = 0.4500E+05
0 Fission Product Concentration =
2.2800E-01 2.2800E-01
2.2800E-01 2.2800E-01
2.2800E-01 2.2800E-01
2.2800E-01 2.2800E-01
0 Fuel Inventory Species Number = 92 Species Name = Moc
0 DZERO = 0.5000E-04 THETA = 0.4500E+05
0 Fission Product Concentration =
1.8800E-01 1.8800E-01
1.8800E-01 1.8800E-01
1.8800E-01 1.8800E-01
1.8800E-01 1.8800E-01
0 Fuel Inventory Species Number = 145 Species Name = Ruc
0 DZERO = 0.5000E-04 THETA = 0.4500E+05
0 Fission Product Concentration =
1.3200E-01 1.3200E-01
1.3200E-01 1.3200E-01
1.3200E-01 1.3200E-01
1.3200E-01 1.3200E-01
0 Fuel Inventory Species Number = 150 Species Name = Sbc
0 DZERO = 0.5000E-04 THETA = 0.4500E+05
0 Fission Product Concentration =
9.0000E-04 9.0000E-04
9.0000E-04 9.0000E-04
9.0000E-04 9.0000E-04
9.0000E-04 9.0000E-04
0 Fuel Inventory Species Number = 157 Species Name = Euc
0 DZERO = 0.5000E-04 THETA = 0.4500E+05
0 Fission Product Concentration =
5.7000E-03 5.7000E-03
5.7000E-03 5.7000E-03
5.7000E-03 5.7000E-03
5.7000E-03 5.7000E-03
0 ***** Grain diameters (m) *****
1.0000E-05 1.0000E-05
1.0000E-05 1.0000E-05
1.0000E-05 1.0000E-05
1.0000E-05 1.0000E-05
1
1998 Victoria 2.0 1 Jul
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```

```

**CORODATA
0 ***** Control Rod Data *****
Absorber diameter = 8.6600E-03
Absorber length = 9.0000E-01
Rod Internal diameter = 8.7000E-03
Rod external diameter = 9.7000E-03
Rod length = 1.0000E+00
Silver mole fraction = 8.0000E-01
Indium mole fraction = 1.5000E-01
Cadmium mole fraction = 5.0000E-02
Initial helium pressure = 1.5000E+05
Control rods per cell = 1. 1. 0. 0. 0. 0. 1. 1. 0. 0. 0. 0.

```

```

**STRUDATA
0 ***** Volume Identification Flags *****
Radial ring number = 1
Ident flags = 0 0 0 3 4 2
0 ***** Steam Separator, Axial level = 4
Vortex Tube Length = 0.5000E-01 , Vortex Tube Radius = 0.1500E+00 , Vane Angle = 0.5200E+00
0 ***** Steam Dryer, Axial level = 5
Number of Bends = 5 , Bend Angle = 0.1040E+01 Bend Pitch = 0.1500E+01
0 ***** Pipe Contraction, Axial level = 6
Entrance Diameter = 0.7000E+00 , Outlet Diameter = 0.3500E+00
0 ***** Volume Identification Flags *****

```

Description of VICTORIA Output

```
Radial ring number = 2
Ident flags = 1 0 0 3 4 1
0 ***** Steam Separator, Axial level = 4
Vortex Tube Length = 0.5000E-01 , Vortex Tube Radius = 0.1500E+00 , Vane Angle = 0.5200E+00
0 ***** Steam Dryer, Axial level = 5
Number of Bends = 5 , Bend Angle = 0.1040E+01 Bend Pitch = 0.1500E+01
0 ***** Settling Flags *****
Radial ring number = 1
Settling flags = -1. -1. -1. -1. -1. -1.
0 ***** Settling Flags *****
Radial ring number = 2
Settling flags = -1. -1. -1. -1. -1. -1.
1
1998 Test Problem (NEB) Victoria 2.0 1 Jul
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0 ***** Axial Flow Areas *****
Radial ring number = 1
Flow areas =
0.1492E+01 0.1492E+01 0.1539E+01 0.1539E+01 0.1539E+01 0.3848E+00
0 ***** Axial Flow Areas *****
Radial ring number = 2
Flow areas =
0.1555E+01 0.1555E+01 0.1602E+01 0.1602E+01 0.1602E+01 0.0000E+00
0 ***** Radial Flow Areas *****
Radial ring number = 1
Flow areas =
2.1991E+00 2.1991E+00 2.1991E+00 2.1991E+00 2.1991E+00 2.1991E+00
0 ***** Radial Flow Areas *****
Radial ring number = 2
Flow areas =
0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
0 ***** Cell Hydraulic Diameters *****
Hydraulic diameters =
0.3630E+00 0.3630E+00 0.1400E+01 0.1400E+01 0.1400E+01 0.1400E+01 0.2757E+00 0.2757E+00
0.1020E+01 0.1020E+01
0.1020E+01 0.1020E+01
0 ***** Cell Floor Areas *****
Floor areas =
0.1155E+01 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.1602E+01 0.0000E+00
0.0000E+00 0.0000E+00
0.0000E+00 0.0000E+00
0 ***** Cell Wall Areas *****
Wall areas =
0.1000E+00 0.1000E+00 0.1000E+00 0.1000E+00 0.1000E+00 0.1000E+00 0.3142E+01 0.3142E+01
0.3142E+01 0.3142E+01
0.3142E+01 0.3142E+01
0 ***** Cell Ceiling Areas *****
Ceiling areas =
0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.1155E+01 0.0000E+00 0.0000E+00
0.0000E+00 0.0000E+00
0.0000E+00 0.1602E+01
0 ***** Structure Identification Flags *****
Structure flags =
0 0 0 0 0 0 1 2 3 4 5 6

**CONTDATA
1
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0 ***** Continuity Input Data *****
Number of species = 1
0 Species number = 32 Species name = H2Og
0 Radial ring number = 1
Species concentrations =
0.3248E+01 0.3248E+01 0.3248E+01 0.3248E+01 0.3248E+01 0.3248E+01
0 Radial ring number = 2
Species concentrations =
0.3248E+01 0.3248E+01 0.3248E+01 0.3248E+01 0.3248E+01 0.3248E+01
```

Description of VICTORIA Output

```

**DECAY
0      idecay = 2
0      Ambient temperature outside insulation (K) =
      3.0000E+02
0      Elapsed time since reactor SCRAM (s) =
      0.0000E+00
0      Reactor power prior to SCRAM (kW) =
      1.0000E+01
0      Structure failure temperature (K) =
      2.5000E+03

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0      Heat-up flags for each bound. pt. =
      0 0 0 0 0 0 1 1 0 0
0      Heat-up flags for each bound. pt. =
      1 1 1 1 1 1
0      Structure wall thickness for each bound. pt. =
      5.0000E-03 5.0000E-03 5.0000E-03 5.0000E-03 5.0000E-03 5.0000E-03 5.0000E-03 5.0000E-03
5.0000E-03 5.0000E-03
      5.0000E-03 5.0000E-03 5.0000E-03 5.0000E-03 5.0000E-03 5.0000E-03
0      Insulation thermal conductivity for each bound. pt. =
      1.0000E-03 1.0000E-03 1.0000E-03 1.0000E-03 1.0000E-03 1.0000E-03 1.0000E-03 1.0000E-03
1.0000E-03 1.0000E-03
      1.0000E-03 1.0000E-03 1.0000E-03 1.0000E-03 1.0000E-03 1.0000E-03
0      Insulation thickness for each bound. pt. =
      5.0000E-02 5.0000E-02 5.0000E-02 5.0000E-02 5.0000E-02 5.0000E-02 5.0000E-02 5.0000E-02
5.0000E-02 5.0000E-02
      5.0000E-02 5.0000E-02 5.0000E-02 5.0000E-02 5.0000E-02 5.0000E-02

**AERODATA
0      ***** Aerosol Input Data *****
0      ncoll = 0 spcing = 0.1000E+02
0      xmlowr = 0.1000E-21 xmuppr = 0.1000E-10
0      nfelem = 2
0      epsa = 0.1000E-05 maxtry = 10
0      cshpfc = 0.1000E+01 dshpfc = 0.1000E+01 stkeff = 0.1000E+01
0      akn = 0.1250E+01 qkn = 0.4100E+00 bkn = 0.8800E+00
0      cm = 0.1140E+01 cs = 0.1170E+01 ct = 0.2180E+01

1
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**PAUSE
0 Ring Level Outer Radial Upper Axial Z-Flow Area R-Flow Area Hydraul. dia Flow Volume Fuel Volume Strc
Area C-Rod Area
(m) (m) (sq m) (sq m) (m) (cu m) (cu m) (sq
m) (sq m)
1 1 7.00000E-01 5.00000E-01 1.49210E+00 2.19910E+00 3.63000E-01 7.69333E-01 1.93221E-04
1.25450E+00 1.52367E-02
1 2 7.00000E-01 1.00000E+00 1.49210E+00 2.19910E+00 3.63000E-01 7.69448E-01 1.93221E-04
1.00000E-01 1.52367E-02
1 3 7.00000E-01 1.50000E+00 1.53940E+00 2.19910E+00 1.40000E+00 7.69680E-01 0.00000E+00
1.00000E-01 0.00000E+00
1 4 7.00000E-01 2.00000E+00 1.53940E+00 2.19910E+00 1.40000E+00 7.69680E-01 0.00000E+00
1.00000E-01 0.00000E+00
1 5 7.00000E-01 2.50000E+00 1.53940E+00 2.19910E+00 1.40000E+00 7.69680E-01 0.00000E+00
1.00000E-01 0.00000E+00
1 6 7.00000E-01 3.00000E+00 3.84800E-01 2.19910E+00 1.40000E+00 7.69565E-01 0.00000E+00
1.25450E+00 0.00000E+00
2 1 1.00000E+00 5.00000E-01 1.55490E+00 0.00000E+00 2.75700E-01 8.00400E-01 1.93221E-04
4.74380E+00 1.52367E-02
2 2 1.00000E+00 1.00000E+00 1.55490E+00 0.00000E+00 2.75700E-01 8.00560E-01 1.93221E-04
3.14160E+00 1.52367E-02

```

Description of VICTORIA Output

```

      2      3      1.00000E+00      1.50000E+00      1.60220E+00      0.00000E+00      1.02000E+00      8.00792E-01      0.00000E+00
3.14160E+00      0.00000E+00
      2      4      1.00000E+00      2.00000E+00      1.60220E+00      0.00000E+00      1.02000E+00      8.00792E-01      0.00000E+00
3.14160E+00      0.00000E+00
      2      5      1.00000E+00      2.50000E+00      1.60220E+00      0.00000E+00      1.02000E+00      8.00792E-01      0.00000E+00
3.14160E+00      0.00000E+00
      2      6      1.00000E+00      3.00000E+00      0.00000E+00      0.00000E+00      1.02000E+00      8.00632E-01      0.00000E+00
4.74380E+00      0.00000E+00

```

```

**TDEPCHEM
0 ***** Control Data Numerical Methods in Chemistry *****

```

```

      igsmax =      200
      epsc =    0.1000E-07
      igsyc =      20
0      Gas Properties Mixing Option =      1

      Frozen Chemistry Option =      0

```

```

**TDEPFUEL
0 Fuel temperature interpolation parameter = 1.000
0 ***** Thermal Hydraulic Data *****

```

```

      Number of time values = 15
0      Clad failure temperature = 2000.0000
      Fully oxidized clad porosity = 0.0500
      Clad melting temperature = 2100.0000

```

```

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```

0	Ring	Level	Time (s)	In Fuel T (K)	Out Fuel T (K)	Cladding T (K)	Fuel Power (kW/m)
	1	1	0.00	1050.	1025.	1000.	0.00
	1	1	50.00	1750.	1725.	1700.	0.00
	1	1	150.00	1750.	1725.	1700.	0.00
	1	1	200.00	1750.	1725.	1700.	0.00
	1	1	250.00	2050.	2025.	2000.	0.00
	1	1	300.00	2050.	2025.	2000.	0.00
	1	1	350.00	2250.	2225.	2200.	0.00
	1	1	400.00	2550.	2525.	2500.	0.00
	1	1	900.00	2550.	2525.	2500.	0.00
	1	1	1000.00	1050.	1025.	1000.	0.00
	1	1	1050.00	1050.	1025.	1000.	0.00
	1	1	1100.00	1050.	1025.	1000.	0.00
	1	1	1150.00	1050.	1025.	1000.	0.00
	1	1	1200.00	1050.	1025.	1000.	0.00
	1	1	1250.00	1050.	1025.	1000.	0.00
	1	2	0.00	1050.	1025.	1000.	0.00
	1	2	50.00	1650.	1625.	1600.	0.00
	1	2	150.00	1650.	1625.	1600.	0.00
	1	2	200.00	1650.	1625.	1600.	0.00
	1	2	250.00	1950.	1925.	1900.	0.00
	1	2	300.00	1950.	1925.	1900.	0.00
	1	2	350.00	2150.	2125.	2100.	0.00
	1	2	400.00	2450.	2425.	2400.	0.00
	1	2	900.00	2450.	2425.	2400.	0.00
	1	2	1000.00	1050.	1025.	1000.	0.00
	1	2	1050.00	1050.	1025.	1000.	0.00
	1	2	1100.00	1050.	1025.	1000.	0.00
	1	2	1150.00	1050.	1025.	1000.	0.00
	1	2	1200.00	1050.	1025.	1000.	0.00
	1	2	1250.00	1050.	1025.	1000.	0.00
	2	1	0.00	1050.	1025.	1000.	0.00
	2	1	50.00	1250.	1225.	1200.	0.00
	2	1	150.00	1250.	1225.	1200.	0.00
	2	1	200.00	1250.	1225.	1200.	0.00
	2	1	250.00	1550.	1525.	1500.	0.00
	2	1	300.00	1550.	1525.	1500.	0.00
	2	1	350.00	1750.	1725.	1700.	0.00
	2	1	400.00	2050.	2025.	2000.	0.00
	2	1	900.00	2050.	2025.	2000.	0.00

Description of VICTORIA Output

2	1	1000.00	1050.	1025.	1000.	0.00
2	1	1050.00	1050.	1025.	1000.	0.00
2	1	1100.00	1050.	1025.	1000.	0.00
2	1	1150.00	1050.	1025.	1000.	0.00
2	1	1200.00	1050.	1025.	1000.	0.00
2	1	1250.00	1050.	1025.	1000.	0.00

1
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Test Problem (NEB)

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0 Ring	Level	Time (s)	In Fuel T (K)	Out Fuel T (K)	Cladding T (K)	Fuel Power (kW/m)
2	2	0.00	1050.	1025.	1000.	0.00
2	2	50.00	1150.	1125.	1100.	0.00
2	2	150.00	1150.	1125.	1100.	0.00
2	2	200.00	1150.	1125.	1100.	0.00
2	2	250.00	1450.	1425.	1400.	0.00
2	2	300.00	1450.	1425.	1400.	0.00
2	2	350.00	1650.	1625.	1600.	0.00
2	2	400.00	1950.	1925.	1900.	0.00
2	2	900.00	1950.	1925.	1900.	0.00
2	2	1000.00	1050.	1025.	1000.	0.00
2	2	1050.00	1050.	1025.	1000.	0.00
2	2	1100.00	1050.	1025.	1000.	0.00
2	2	1150.00	1050.	1025.	1000.	0.00
2	2	1200.00	1050.	1025.	1000.	0.00
2	2	1250.00	1050.	1025.	1000.	0.00

**TDEPSTRU

0 Ring	Level	Time (s)	Gas Temp. (K)
1	1	0.00	1000.
1	1	50.00	1600.
1	1	150.00	1600.
1	1	200.00	1600.
1	1	250.00	1900.
1	1	300.00	1900.
1	1	350.00	2100.
1	1	400.00	2400.
1	1	900.00	2400.
1	1	1000.00	750.
1	1	1050.00	750.
1	1	1100.00	750.
1	1	1150.00	750.
1	1	1200.00	750.
1	1	1250.00	750.
1	2	0.00	1000.
1	2	50.00	1500.
1	2	150.00	1500.
1	2	200.00	1500.
1	2	250.00	1800.
1	2	300.00	1800.
1	2	350.00	2000.
1	2	400.00	2300.
1	2	900.00	2300.
1	2	1000.00	750.
1	2	1050.00	750.
1	2	1100.00	750.
1	2	1150.00	750.
1	2	1200.00	750.
1	2	1250.00	750.

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Test Problem (NEB)

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0 Ring	Level	Time (s)	Gas Temp. (K)
1	3	0.00	1000.
1	3	50.00	1400.
1	3	150.00	1400.
1	3	200.00	1400.
1	3	250.00	1700.
1	3	300.00	1700.
1	3	350.00	1900.
1	3	400.00	2200.

Description of VICTORIA Output

1	3	900.00	2200.
1	3	1000.00	750.
1	3	1050.00	750.
1	3	1100.00	750.
1	3	1150.00	750.
1	3	1200.00	750.
1	3	1250.00	750.
1	4	0.00	1000.
1	4	50.00	1300.
1	4	150.00	1300.
1	4	200.00	1300.
1	4	250.00	1600.
1	4	300.00	1600.
1	4	350.00	1800.
1	4	400.00	2100.
1	4	900.00	2100.
1	4	1000.00	750.
1	4	1050.00	750.
1	4	1100.00	750.
1	4	1150.00	750.
1	4	1200.00	750.
1	4	1250.00	750.
1	5	0.00	1000.
1	5	50.00	1200.
1	5	150.00	1200.
1	5	200.00	1200.
1	5	250.00	1500.
1	5	300.00	1500.
1	5	350.00	1700.
1	5	400.00	2000.
1	5	900.00	2000.
1	5	1000.00	750.
1	5	1050.00	750.
1	5	1100.00	750.
1	5	1150.00	750.
1	5	1200.00	750.
1	5	1250.00	750.
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Test Problem (NEB)			Victoria 2.0 1 Jul
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0 Ring	Level	Time (s)	Gas Temp. (K)
1	6	0.00	1000.
1	6	50.00	1100.
1	6	150.00	1100.
1	6	200.00	1100.
1	6	250.00	1400.
1	6	300.00	1400.
1	6	350.00	1600.
1	6	400.00	1900.
1	6	900.00	1900.
1	6	1000.00	750.
1	6	1050.00	750.
1	6	1100.00	750.
1	6	1150.00	750.
1	6	1200.00	750.
1	6	1250.00	750.
2	1	0.00	1000.
2	1	50.00	1100.
2	1	150.00	1100.
2	1	200.00	1100.
2	1	250.00	1400.
2	1	300.00	1400.
2	1	350.00	1600.
2	1	400.00	1900.
2	1	900.00	1900.
2	1	1000.00	750.
2	1	1050.00	750.
2	1	1100.00	750.
2	1	1150.00	750.
2	1	1200.00	750.
2	1	1250.00	750.
2	2	0.00	1000.
2	2	50.00	1000.
2	2	150.00	1000.

Description of VICTORIA Output

2	2	200.00	1000.
2	2	250.00	1300.
2	2	300.00	1300.
2	2	350.00	1500.
2	2	400.00	1800.
2	2	900.00	1800.
2	2	1000.00	750.
2	2	1050.00	750.
2	2	1100.00	750.
2	2	1150.00	750.
2	2	1200.00	750.
2	2	1250.00	750.

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Test Problem (NEB)
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0 Ring	Level	Time (s)	Gas Temp. (K)
2	3	0.00	1000.
2	3	50.00	1000.
2	3	150.00	1000.
2	3	200.00	1000.
2	3	250.00	1200.
2	3	300.00	1200.
2	3	350.00	1400.
2	3	400.00	1700.
2	3	900.00	1700.
2	3	1000.00	750.
2	3	1050.00	750.
2	3	1100.00	750.
2	3	1150.00	750.
2	3	1200.00	750.
2	3	1250.00	750.
2	4	0.00	1000.
2	4	50.00	1000.
2	4	150.00	1000.
2	4	200.00	1000.
2	4	250.00	1100.
2	4	300.00	1100.
2	4	350.00	1300.
2	4	400.00	1600.
2	4	900.00	1600.
2	4	1000.00	750.
2	4	1050.00	750.
2	4	1100.00	750.
2	4	1150.00	750.
2	4	1200.00	750.
2	4	1250.00	750.
2	5	0.00	1000.
2	5	50.00	1000.
2	5	150.00	1000.
2	5	200.00	1000.
2	5	250.00	1000.
2	5	300.00	1000.
2	5	350.00	1200.
2	5	400.00	1500.
2	5	900.00	1500.
2	5	1000.00	750.
2	5	1050.00	750.
2	5	1100.00	750.
2	5	1150.00	750.
2	5	1200.00	750.
2	5	1250.00	750.

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Test Problem (NEB)
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0 Ring	Level	Time (s)	Gas Temp. (K)
2	6	0.00	1000.
2	6	50.00	1000.
2	6	150.00	1000.
2	6	200.00	1000.
2	6	250.00	1000.
2	6	300.00	1000.
2	6	350.00	1100.

Description of VICTORIA Output

2	6	400.00	1400.		
2	6	900.00	1400.		
2	6	1000.00	750.		
2	6	1050.00	750.		
2	6	1100.00	750.		
2	6	1150.00	750.		
2	6	1200.00	750.		
2	6	1250.00	750.		
0 Ring	Level	Time (s)	Ceiling T (K)	Wall T (K)	Floor T (K)
1	1	0.00	1000.	1000.	1000.
1	1	50.00	1500.	1500.	1500.
1	1	150.00	1500.	1500.	1500.
1	1	200.00	1500.	1500.	1500.
1	1	250.00	1800.	1800.	1800.
1	1	300.00	1800.	1800.	1800.
1	1	350.00	2000.	2000.	2000.
1	1	400.00	2300.	2300.	2300.
1	1	900.00	2300.	2300.	2300.
1	1	1000.00	750.	750.	750.
1	1	1050.00	750.	750.	750.
1	1	1100.00	750.	750.	750.
1	1	1150.00	750.	750.	750.
1	1	1200.00	750.	750.	750.
1	1	1250.00	750.	750.	750.
1	2	0.00	1000.	1000.	1000.
1	2	50.00	1400.	1400.	1400.
1	2	150.00	1400.	1400.	1400.
1	2	200.00	1400.	1400.	1400.
1	2	250.00	1700.	1700.	1700.
1	2	300.00	1700.	1700.	1700.
1	2	350.00	1900.	1900.	1900.
1	2	400.00	2200.	2200.	2200.
1	2	900.00	2200.	2200.	2200.
1	2	1000.00	750.	750.	750.
1	2	1050.00	750.	750.	750.
1	2	1100.00	750.	750.	750.
1	2	1150.00	750.	750.	750.
1	2	1200.00	750.	750.	750.
1	2	1250.00	750.	750.	750.

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Test Problem (NEB)

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0 Ring	Level	Time (s)	Ceiling T (K)	Wall T (K)	Floor T (K)
1	3	0.00	1000.	1000.	1000.
1	3	50.00	1300.	1300.	1300.
1	3	150.00	1300.	1300.	1300.
1	3	200.00	1300.	1300.	1300.
1	3	250.00	1600.	1600.	1600.
1	3	300.00	1600.	1600.	1600.
1	3	350.00	1800.	1800.	1800.
1	3	400.00	2100.	2100.	2100.
1	3	900.00	2100.	2100.	2100.
1	3	1000.00	750.	750.	750.
1	3	1050.00	750.	750.	750.
1	3	1100.00	750.	750.	750.
1	3	1150.00	750.	750.	750.
1	3	1200.00	750.	750.	750.
1	3	1250.00	750.	750.	750.
1	4	0.00	1000.	1000.	1000.
1	4	50.00	1200.	1200.	1200.
1	4	150.00	1200.	1200.	1200.
1	4	200.00	1200.	1200.	1200.
1	4	250.00	1500.	1500.	1500.
1	4	300.00	1500.	1500.	1500.
1	4	350.00	1700.	1700.	1700.
1	4	400.00	2000.	2000.	2000.
1	4	900.00	2000.	2000.	2000.
1	4	1000.00	750.	750.	750.
1	4	1050.00	750.	750.	750.
1	4	1100.00	750.	750.	750.
1	4	1150.00	750.	750.	750.
1	4	1200.00	750.	750.	750.
1	4	1250.00	750.	750.	750.
1	5	0.00	1000.	1000.	1000.

Description of VICTORIA Output

1	5	50.00	1100.	1100.	1100.
1	5	150.00	1100.	1100.	1100.
1	5	200.00	1100.	1100.	1100.
1	5	250.00	1400.	1400.	1400.
1	5	300.00	1400.	1400.	1400.
1	5	350.00	1600.	1600.	1600.
1	5	400.00	1900.	1900.	1900.
1	5	900.00	1900.	1900.	1900.
1	5	1000.00	750.	750.	750.
1	5	1050.00	750.	750.	750.
1	5	1100.00	750.	750.	750.
1	5	1150.00	750.	750.	750.
1	5	1200.00	750.	750.	750.
1	5	1250.00	750.	750.	750.

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Test Problem (NEB)
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0 Ring	Level	Time (s)	Ceiling T (K)	Wall T (K)	Floor T (K)
1	6	0.00	1000.	1000.	1000.
1	6	50.00	1000.	1000.	1000.
1	6	150.00	1000.	1000.	1000.
1	6	200.00	1000.	1000.	1000.
1	6	250.00	1300.	1300.	1300.
1	6	300.00	1300.	1300.	1300.
1	6	350.00	1500.	1500.	1500.
1	6	400.00	1800.	1800.	1800.
1	6	900.00	1800.	1800.	1800.
1	6	1000.00	750.	750.	750.
1	6	1050.00	750.	750.	750.
1	6	1100.00	750.	750.	750.
1	6	1150.00	750.	750.	750.
1	6	1200.00	750.	750.	750.
1	6	1250.00	750.	750.	750.
2	1	0.00	1000.	1000.	1000.
2	1	50.00	1000.	1000.	1000.
2	1	150.00	1000.	1000.	1000.
2	1	200.00	1000.	1000.	1000.
2	1	250.00	1300.	1300.	1300.
2	1	300.00	1300.	1300.	1300.
2	1	350.00	1500.	1500.	1500.
2	1	400.00	1800.	1800.	1800.
2	1	900.00	1800.	1800.	1800.
2	1	1000.00	750.	750.	750.
2	1	1050.00	750.	750.	750.
2	1	1100.00	750.	750.	750.
2	1	1150.00	750.	750.	750.
2	1	1200.00	750.	750.	750.
2	1	1250.00	750.	750.	750.
2	2	0.00	1000.	1000.	1000.
2	2	50.00	1000.	1000.	1000.
2	2	150.00	1000.	1000.	1000.
2	2	200.00	1000.	1000.	1000.
2	2	250.00	1200.	1200.	1200.
2	2	300.00	1200.	1200.	1200.
2	2	350.00	1400.	1400.	1400.
2	2	400.00	1700.	1700.	1700.
2	2	900.00	1700.	1700.	1700.
2	2	1000.00	750.	750.	750.
2	2	1050.00	750.	750.	750.
2	2	1100.00	750.	750.	750.
2	2	1150.00	750.	750.	750.
2	2	1200.00	750.	750.	750.
2	2	1250.00	750.	750.	750.

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Test Problem (NEB)
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0 Ring	Level	Time (s)	Ceiling T (K)	Wall T (K)	Floor T (K)
2	3	0.00	1000.	1000.	1000.
2	3	50.00	1000.	1000.	1000.
2	3	150.00	1000.	1000.	1000.
2	3	200.00	1000.	1000.	1000.
2	3	250.00	1100.	1100.	1100.

Description of VICTORIA Output

2	3	300.00	1100.	1100.	1100.
2	3	350.00	1300.	1300.	1300.
2	3	400.00	1600.	1600.	1600.
2	3	900.00	1600.	1600.	1600.
2	3	1000.00	750.	750.	750.
2	3	1050.00	750.	750.	750.
2	3	1100.00	750.	750.	750.
2	3	1150.00	750.	750.	750.
2	3	1200.00	750.	750.	750.
2	3	1250.00	750.	750.	750.
2	4	0.00	1000.	1000.	1000.
2	4	50.00	1000.	1000.	1000.
2	4	150.00	1000.	1000.	1000.
2	4	200.00	1000.	1000.	1000.
2	4	250.00	1000.	1000.	1000.
2	4	300.00	1000.	1000.	1000.
2	4	350.00	1200.	1200.	1200.
2	4	400.00	1500.	1500.	1500.
2	4	900.00	1500.	1500.	1500.
2	4	1000.00	750.	750.	750.
2	4	1050.00	750.	750.	750.
2	4	1100.00	750.	750.	750.
2	4	1150.00	750.	750.	750.
2	4	1200.00	750.	750.	750.
2	4	1250.00	750.	750.	750.
2	5	0.00	1000.	1000.	1000.
2	5	50.00	1000.	1000.	1000.
2	5	150.00	1000.	1000.	1000.
2	5	200.00	1000.	1000.	1000.
2	5	250.00	1000.	1000.	1000.
2	5	300.00	1000.	1000.	1000.
2	5	350.00	1100.	1100.	1100.
2	5	400.00	1400.	1400.	1400.
2	5	900.00	1400.	1400.	1400.
2	5	1000.00	750.	750.	750.
2	5	1050.00	750.	750.	750.
2	5	1100.00	750.	750.	750.
2	5	1150.00	750.	750.	750.
2	5	1200.00	750.	750.	750.
2	5	1250.00	750.	750.	750.

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0 Ring	Level	Time (s)	Ceiling T (K)	Wall T (K)	Floor T (K)
2	6	0.00	1000.	1000.	1000.
2	6	50.00	1000.	1000.	1000.
2	6	150.00	1000.	1000.	1000.
2	6	200.00	1000.	1000.	1000.
2	6	250.00	1000.	1000.	1000.
2	6	300.00	1000.	1000.	1000.
2	6	350.00	1000.	1000.	1000.
2	6	400.00	1300.	1300.	1300.
2	6	900.00	1300.	1300.	1300.
2	6	1000.00	750.	750.	750.
2	6	1050.00	750.	750.	750.
2	6	1100.00	750.	750.	750.
2	6	1150.00	750.	750.	750.
2	6	1200.00	750.	750.	750.
2	6	1250.00	750.	750.	750.

0 Ring	Level	Time (s)	Pressures (Pa)
1	1	0.00	1.50000E+06
1	1	50.00	1.50000E+06
1	1	150.00	1.50000E+06
1	1	200.00	1.50000E+06
1	1	250.00	1.50000E+06
1	1	300.00	1.50000E+06
1	1	350.00	1.50000E+06
1	1	400.00	1.50000E+06
1	1	900.00	1.50000E+05
1	1	1000.00	1.50000E+05
1	1	1050.00	1.50000E+05
1	1	1100.00	1.50000E+05
1	1	1150.00	1.50000E+05
1	1	1200.00	1.50000E+05

Description of VICTORIA Output

1	1	1250.00	1.50000E+05
1	2	0.00	1.50000E+06
1	2	50.00	1.50000E+06
1	2	150.00	1.50000E+06
1	2	200.00	1.50000E+06
1	2	250.00	1.50000E+06
1	2	300.00	1.50000E+06
1	2	350.00	1.50000E+06
1	2	400.00	1.50000E+06
1	2	900.00	1.50000E+05
1	2	1000.00	1.50000E+05
1	2	1050.00	1.50000E+05
1	2	1100.00	1.50000E+05
1	2	1150.00	1.50000E+05
1	2	1200.00	1.50000E+05
1	2	1250.00	1.50000E+05

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0 Ring	Level	Time (s)	Pressures (Pa)
1	3	0.00	1.50000E+06
1	3	50.00	1.50000E+06
1	3	150.00	1.50000E+06
1	3	200.00	1.50000E+06
1	3	250.00	1.50000E+06
1	3	300.00	1.50000E+06
1	3	350.00	1.50000E+06
1	3	400.00	1.50000E+06
1	3	900.00	1.50000E+05
1	3	1000.00	1.50000E+05
1	3	1050.00	1.50000E+05
1	3	1100.00	1.50000E+05
1	3	1150.00	1.50000E+05
1	3	1200.00	1.50000E+05
1	3	1250.00	1.50000E+05
1	4	0.00	1.50000E+06
1	4	50.00	1.50000E+06
1	4	150.00	1.50000E+06
1	4	200.00	1.50000E+06
1	4	250.00	1.50000E+06
1	4	300.00	1.50000E+06
1	4	350.00	1.50000E+06
1	4	400.00	1.50000E+06
1	4	900.00	1.50000E+05
1	4	1000.00	1.50000E+05
1	4	1050.00	1.50000E+05
1	4	1100.00	1.50000E+05
1	4	1150.00	1.50000E+05
1	4	1200.00	1.50000E+05
1	4	1250.00	1.50000E+05
1	5	0.00	1.50000E+06
1	5	50.00	1.50000E+06
1	5	150.00	1.50000E+06
1	5	200.00	1.50000E+06
1	5	250.00	1.50000E+06
1	5	300.00	1.50000E+06
1	5	350.00	1.50000E+06
1	5	400.00	1.50000E+06
1	5	900.00	1.50000E+05
1	5	1000.00	1.50000E+05
1	5	1050.00	1.50000E+05
1	5	1100.00	1.50000E+05
1	5	1150.00	1.50000E+05
1	5	1200.00	1.50000E+05
1	5	1250.00	1.50000E+05

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0 Ring	Level	Time (s)	Pressures (Pa)
1	6	0.00	1.50000E+06
1	6	50.00	1.50000E+06
1	6	150.00	1.50000E+06

Description of VICTORIA Output

1	6	200.00	1.50000E+06
1	6	250.00	1.50000E+06
1	6	300.00	1.50000E+06
1	6	350.00	1.50000E+06
1	6	400.00	1.50000E+06
1	6	900.00	1.50000E+05
1	6	1000.00	1.50000E+05
1	6	1050.00	1.50000E+05
1	6	1100.00	1.50000E+05
1	6	1150.00	1.50000E+05
1	6	1200.00	1.50000E+05
1	6	1250.00	1.50000E+05
2	1	0.00	1.50000E+06
2	1	50.00	1.50000E+06
2	1	150.00	1.50000E+06
2	1	200.00	1.50000E+06
2	1	250.00	1.50000E+06
2	1	300.00	1.50000E+06
2	1	350.00	1.50000E+06
2	1	400.00	1.50000E+06
2	1	900.00	1.50000E+05
2	1	1000.00	1.50000E+05
2	1	1050.00	1.50000E+05
2	1	1100.00	1.50000E+05
2	1	1150.00	1.50000E+05
2	1	1200.00	1.50000E+05
2	1	1250.00	1.50000E+05
2	2	0.00	1.50000E+06
2	2	50.00	1.50000E+06
2	2	150.00	1.50000E+06
2	2	200.00	1.50000E+06
2	2	250.00	1.50000E+06
2	2	300.00	1.50000E+06
2	2	350.00	1.50000E+06
2	2	400.00	1.50000E+06
2	2	900.00	1.50000E+05
2	2	1000.00	1.50000E+05
2	2	1050.00	1.50000E+05
2	2	1100.00	1.50000E+05
2	2	1150.00	1.50000E+05
2	2	1200.00	1.50000E+05
2	2	1250.00	1.50000E+05

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0 Ring	Level	Time (s)	Pressures (Pa)
2	3	0.00	1.50000E+06
2	3	50.00	1.50000E+06
2	3	150.00	1.50000E+06
2	3	200.00	1.50000E+06
2	3	250.00	1.50000E+06
2	3	300.00	1.50000E+06
2	3	350.00	1.50000E+06
2	3	400.00	1.50000E+06
2	3	900.00	1.50000E+05
2	3	1000.00	1.50000E+05
2	3	1050.00	1.50000E+05
2	3	1100.00	1.50000E+05
2	3	1150.00	1.50000E+05
2	3	1200.00	1.50000E+05
2	3	1250.00	1.50000E+05
2	4	0.00	1.50000E+06
2	4	50.00	1.50000E+06
2	4	150.00	1.50000E+06
2	4	200.00	1.50000E+06
2	4	250.00	1.50000E+06
2	4	300.00	1.50000E+06
2	4	350.00	1.50000E+06
2	4	400.00	1.50000E+06
2	4	900.00	1.50000E+05
2	4	1000.00	1.50000E+05
2	4	1050.00	1.50000E+05
2	4	1100.00	1.50000E+05
2	4	1150.00	1.50000E+05

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2	4	1200.00	1.50000E+05
2	4	1250.00	1.50000E+05
2	5	0.00	1.50000E+06
2	5	50.00	1.50000E+06
2	5	150.00	1.50000E+06
2	5	200.00	1.50000E+06
2	5	250.00	1.50000E+06
2	5	300.00	1.50000E+06
2	5	350.00	1.50000E+06
2	5	400.00	1.50000E+06
2	5	900.00	1.50000E+05
2	5	1000.00	1.50000E+05
2	5	1050.00	1.50000E+05
2	5	1100.00	1.50000E+05
2	5	1150.00	1.50000E+05
2	5	1200.00	1.50000E+05
2	5	1250.00	1.50000E+05

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0 Ring	Level	Time (s)	Pressures (Pa)
2	6	0.00	1.50000E+06
2	6	50.00	1.50000E+06
2	6	150.00	1.50000E+06
2	6	200.00	1.50000E+06
2	6	250.00	1.50000E+06
2	6	300.00	1.50000E+06
2	6	350.00	1.50000E+06
2	6	400.00	1.50000E+06
2	6	900.00	1.50000E+05
2	6	1000.00	1.50000E+05
2	6	1050.00	1.50000E+05
2	6	1100.00	1.50000E+05
2	6	1150.00	1.50000E+05
2	6	1200.00	1.50000E+05
2	6	1250.00	1.50000E+05

0 Ring	Level	Time (s)	Radial V (m/s)	Axial V (m/s)
1	1	0.00	0.17770	0.26190
1	1	50.00	0.28229	0.41604
1	1	150.00	0.28229	0.41604
1	1	200.00	0.05699	0.08400
1	1	250.00	0.06704	0.09881
1	1	300.00	0.06737	0.09929
1	1	350.00	0.07452	0.10984
1	1	400.00	0.08499	0.12526
1	1	900.00	0.08095	0.11931
1	1	1000.00	0.02646	0.03900
1	1	1050.00	0.02646	0.03900
1	1	1100.00	0.13232	0.19502
1	1	1150.00	1.05858	1.56016
1	1	1200.00	1.05858	1.56016
1	1	1250.00	1.05858	1.56016
1	2	0.00	0.00000	0.26524
1	2	50.00	0.00000	0.39004
1	2	150.00	0.00000	0.39004
1	2	200.00	0.00000	0.08042
1	2	250.00	0.00000	0.09361
1	2	300.00	0.00000	0.09506
1	2	350.00	0.00000	0.10591
1	2	400.00	0.00000	0.12094
1	2	900.00	0.00000	0.10401
1	2	1000.00	0.00000	0.03900
1	2	1050.00	0.00000	0.03900
1	2	1100.00	0.00000	0.19502
1	2	1150.00	0.00000	1.56016
1	2	1200.00	0.00000	1.56016
1	2	1250.00	0.00000	1.56016

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0 Ring	Level	Time (s)	Radial V (m/s)	Axial V (m/s)
1	3	0.00	0.00000	0.25994

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1	3	50.00	0.00000	0.35285
1	3	150.00	0.00000	0.35285
1	3	200.00	0.00000	0.07451
1	3	250.00	0.00000	0.08569
1	3	300.00	0.00000	0.08807
1	3	350.00	0.00000	0.09889
1	3	400.00	0.00000	0.11303
1	3	900.00	0.00000	0.08676
1	3	1000.00	0.00000	0.03781
1	3	1050.00	0.00000	0.03781
1	3	1100.00	0.00000	0.18903
1	3	1150.00	0.00000	1.51223
1	3	1200.00	0.00000	1.51223
1	3	1250.00	0.00000	1.51223
1	4	0.00	0.00000	0.26225
1	4	50.00	0.00000	0.32765
1	4	150.00	0.00000	0.32765
1	4	200.00	0.00000	0.07107
1	4	250.00	0.00000	0.08065
1	4	300.00	0.00000	0.08400
1	4	350.00	0.00000	0.09511
1	4	400.00	0.00000	0.10879
1	4	900.00	0.00000	0.07382
1	4	1000.00	0.00000	0.03781
1	4	1050.00	0.00000	0.03781
1	4	1100.00	0.00000	0.18903
1	4	1150.00	0.00000	1.51223
1	4	1200.00	0.00000	1.51223
1	4	1250.00	0.00000	1.51223
1	5	0.00	0.00000	0.26392
1	5	50.00	0.00000	0.30245
1	5	150.00	0.00000	0.30245
1	5	200.00	0.00000	0.06760
1	5	250.00	0.00000	0.07561
1	5	300.00	0.00000	0.07993
1	5	350.00	0.00000	0.09133
1	5	400.00	0.00000	0.10451
1	5	900.00	0.00000	0.06197
1	5	1000.00	0.00000	0.03781
1	5	1050.00	0.00000	0.03781
1	5	1100.00	0.00000	0.18903
1	5	1150.00	0.00000	1.51223
1	5	1200.00	0.00000	1.51223
1	5	1250.00	0.00000	1.51223
1				
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0 Ring	Level	Time (s)	Radial V (m/s)	Axial V (m/s)
1	6	0.00	-0.17835	2.07867
1	6	50.00	-0.17643	2.21822
1	6	150.00	-0.17643	2.21822
1	6	200.00	-0.04051	0.51111
1	6	250.00	-0.03529	0.56464
1	6	300.00	-0.04058	0.62809
1	6	350.00	-0.04573	0.73033
1	6	400.00	-0.05292	0.81127
1	6	900.00	-0.02541	0.40192
1	6	1000.00	-0.02646	0.30248
1	6	1050.00	-0.02646	0.30248
1	6	1100.00	-0.13232	1.51242
1	6	1150.00	-1.05858	12.09938
1	6	1200.00	-1.05858	12.09938
1	6	1250.00	-1.05858	12.09938
2	1	0.00	0.00000	0.25223
2	1	50.00	0.00000	0.27448
2	1	150.00	0.00000	0.27448
2	1	200.00	0.00000	0.05756
2	1	250.00	0.00000	0.06987
2	1	300.00	0.00000	0.07145
2	1	350.00	0.00000	0.08188
2	1	400.00	0.00000	0.09606
2	1	900.00	0.00000	0.08297
2	1	1000.00	0.00000	0.03743
2	1	1050.00	0.00000	0.03743

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2	1	1100.00	0.00000	0.18714
2	1	1150.00	0.00000	1.49715
2	1	1200.00	0.00000	1.49715
2	1	1250.00	0.00000	1.49715
2	2	0.00	0.00000	0.25223
2	2	50.00	0.00000	0.24952
2	2	150.00	0.00000	0.24952
2	2	200.00	0.00000	0.05464
2	2	250.00	0.00000	0.06488
2	2	300.00	0.00000	0.06768
2	2	350.00	0.00000	0.07843
2	2	400.00	0.00000	0.09191
2	2	900.00	0.00000	0.07161
2	2	1000.00	0.00000	0.03743
2	2	1050.00	0.00000	0.03743
2	2	1100.00	0.00000	0.18714
2	2	1150.00	0.00000	1.49715
2	2	1200.00	0.00000	1.49715
2	2	1250.00	0.00000	1.49715

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0 Ring	Level	Time (s)	Radial V (m/s)	Axial V (m/s)
2	3	0.00	0.00000	0.24479
2	3	50.00	0.00000	0.24216
2	3	150.00	0.00000	0.24216
2	3	200.00	0.00000	0.05469
2	3	250.00	0.00000	0.05812
2	3	300.00	0.00000	0.06206
2	3	350.00	0.00000	0.07281
2	3	400.00	0.00000	0.08514
2	3	900.00	0.00000	0.05930
2	3	1000.00	0.00000	0.03632
2	3	1050.00	0.00000	0.03632
2	3	1100.00	0.00000	0.18162
2	3	1150.00	0.00000	1.45295
2	3	1200.00	0.00000	1.45295
2	3	1250.00	0.00000	1.45295
2	4	0.00	0.00000	0.24479
2	4	50.00	0.00000	0.24216
2	4	150.00	0.00000	0.24216
2	4	200.00	0.00000	0.05560
2	4	250.00	0.00000	0.05328
2	4	300.00	0.00000	0.05843
2	4	350.00	0.00000	0.06948
2	4	400.00	0.00000	0.08103
2	4	900.00	0.00000	0.05014
2	4	1000.00	0.00000	0.03632
2	4	1050.00	0.00000	0.03632
2	4	1100.00	0.00000	0.18162
2	4	1150.00	0.00000	1.45295
2	4	1200.00	0.00000	1.45295
2	4	1250.00	0.00000	1.45295
2	5	0.00	0.00000	0.24479
2	5	50.00	0.00000	0.24216
2	5	150.00	0.00000	0.24216
2	5	200.00	0.00000	0.05560
2	5	250.00	0.00000	0.04843
2	5	300.00	0.00000	0.05478
2	5	350.00	0.00000	0.06614
2	5	400.00	0.00000	0.07687
2	5	900.00	0.00000	0.04201
2	5	1000.00	0.00000	0.03632
2	5	1050.00	0.00000	0.03632
2	5	1100.00	0.00000	0.18162
2	5	1150.00	0.00000	1.45295
2	5	1200.00	0.00000	1.45295
2	5	1250.00	0.00000	1.45295

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0 Ring	Level	Time (s)	Radial V (m/s)	Axial V (m/s)
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Description of VICTORIA Output

```

2      6      0.00      0.00000      0.00000
2      6      50.00     0.00000      0.00000
2      6      150.00    0.00000      0.00000
2      6      200.00    0.00000      0.00000
2      6      250.00    0.00000      0.00000
2      6      300.00    0.00000      0.00000
2      6      350.00    0.00000      0.00000
2      6      400.00    0.00000      0.00000
2      6      900.00    0.00000      0.00000
2      6     1000.00    0.00000      0.00000
2      6     1050.00    0.00000      0.00000
2      6     1100.00    0.00000      0.00000
2      6     1150.00    0.00000      0.00000
2      6     1200.00    0.00000      0.00000
2      6     1250.00    0.00000      0.00000

**TDEPSRCE
0      ***** Aerosol Sources *****      Number of sources =      1
0      Number of time values for aerosol sources =      15
0      Time values
0      0.0000E+00  0.5000E+02  0.1500E+03  0.2000E+03  0.2500E+03  0.3000E+03  0.3500E+03  0.4000E+03
0.9000E+03  0.1000E+04
0      Time values
0      0.1050E+04  0.1100E+04  0.1150E+04  0.1200E+04  0.1250E+04
0      Number of species in single-component aerosol source =      2
0      Species number =      1 Species name = CsIc      Mass fraction=      0.5000E+00
0      Species number =      3 Species name = CsOHc      Mass fraction=      0.5000E+00
0      Source input j,i =      1 1
0      aerosol source rate =
0      0.1000E-02  0.1000E-02  0.1000E-02  0.1000E-02  0.1000E-02  0.1000E-02  0.1000E-02  0.1000E-02
0.1000E-02  0.1000E-02
0      aerosol source rate =
0      0.1000E-02  0.1000E-02  0.1000E-02  0.1000E-02  0.1000E-02
0      source gsd =      0.2000E+01 source r50 =      0.5000E-07
0      ***** Fission Product Vapour Sources *****
0      Number of sources =      2
0      Number of time values in source input =      15
0      Time values
0      0.0000E+00  0.5000E+02  0.1500E+03  0.2000E+03  0.2500E+03  0.3000E+03  0.3500E+03  0.4000E+03
0.9000E+03  0.1000E+04
0      Time values
0      0.1050E+04  0.1100E+04  0.1150E+04  0.1200E+04  0.1250E+04

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0      Species number =      32 Species name = H2Og      Cell affected by source (j,i)=      1 1
0      Mass source rate into cell =
0      0.2520E+01  0.2520E+01  0.2520E+01  0.5040E+00  0.5040E+00  0.5040E+00  0.2520E+00  0.2520E+00
0.2520E-01  0.2520E-01
0      Mass source rate into cell =
0      0.2520E-01  0.1260E+00  0.1008E+01  0.2016E+01  0.2016E+01
0      Species number =      31 Species name = H2g      Cell affected by source (j,i)=      1 1
0      Mass source rate into cell =
0      0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.2800E-01  0.2800E-01
0.2800E-02  0.2800E-02
0      Mass source rate into cell =
0      0.2800E-02  0.1400E-01  0.1120E+00  0.0000E+00  0.0000E+00

**TDEPCTRL
0      ***** Time Step Control Data *****

0      Problem start time =      0.00000000E+00 seconds
0      Time step length =      1.00000000E+00 seconds
0      Problem end time =      1.10000000E+03 seconds
0      ***** Output Control Data *****

0      Skip 1100 time steps for printed output
0      Skip 25 time steps for graphical output
0      Output type =      0
0      0 = full output, all cells

```

Description of VICTORIA Output

```
-1 = full output, specified cells
(-) 2 = aerosol output only
(-) 3 = chemistry output only
(-)>3 = temp/pressures/mass output only
<= -1 = specify cell numbers on next line
Do/do not (1/0) - write restart dump          1
0      Write restart dump on file test.rst
```

7.1.4 Temperatures and Pressures

Temperatures and pressures for each node are written in tabular form for each node, as shown on the following page. These data are not calculated by VICTORIA, but are interpolated from the thermal-hydraulic input data described in Subsections 6.5.2 and 6.5.3. This output is included because it is often useful to know precisely what conditions prevail at the current time step.

For this example, the temperatures correspond to the inner and outer fuel nodes; the fuel cladding; the bulk gas; the film or layer of deposits on the surface of structural surfaces; the average for all structures; and surfaces that are oriented as ceilings, walls, and floors.

7.1.5 Bulk Gas Transport Properties

Bulk gas transport properties are also written for each node in tabular form, as shown on the following page. Some of these values are taken from the input thermal-hydraulic data described in Subsection 6.5.3; some are calculated by VICTORIA. The first column of data contains the calculated Reynolds numbers. The second and third columns contain the axial and radial velocities, which are interpolated from the input data. Following this are the calculated momentum and boundary-layer thicknesses for structure and fuel surfaces. The final three columns contain bulk gas density, thermal conductivity, and viscosity.

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temperatures (K) and pressures (Pa) at time = 1.25000E+03 s

i, j	fuel temp.	fuel temp.	clad temp.	gas temp.	gas press.	film temp.	strc. temp.	ceill. temp.	wall temp.	floor temp.
1, 1	1.044E+03	1.031E+03	1.000E+03	7.500E+02	1.500E+05	7.500E+02	7.500E+02	7.500E+02	7.500E+02	7.500E+02
1, 2	1.044E+03	1.031E+03	1.000E+03	7.500E+02	1.500E+05	7.500E+02	7.500E+02	7.500E+02	7.500E+02	7.500E+02
1, 3				7.500E+02	1.500E+05	7.500E+02	7.500E+02	7.500E+02	7.500E+02	7.500E+02
1, 4				7.500E+02	1.500E+05	7.500E+02	7.500E+02	7.500E+02	7.500E+02	7.500E+02
1, 5				7.500E+02	1.500E+05	7.500E+02	7.500E+02	7.500E+02	7.500E+02	7.500E+02
1, 6				7.500E+02	1.500E+05	1.464E+03	1.472E+03	1.472E+03	1.472E+03	1.472E+03
2, 1	1.044E+03	1.031E+03	1.000E+03	7.500E+02	1.500E+05	1.489E+03	1.492E+03	1.492E+03	1.492E+03	1.492E+03
2, 2	1.044E+03	1.031E+03	1.000E+03	7.500E+02	1.500E+05	1.328E+03	1.330E+03	1.330E+03	1.330E+03	1.330E+03
2, 3				7.500E+02	1.500E+05	1.285E+03	1.288E+03	1.288E+03	1.288E+03	1.288E+03
2, 4				7.500E+02	1.500E+05	1.202E+03	1.205E+03	1.205E+03	1.205E+03	1.205E+03
2, 5				7.500E+02	1.500E+05	1.162E+03	1.164E+03	1.164E+03	1.164E+03	1.164E+03
2, 6				7.500E+02	1.500E+05	1.059E+03	1.063E+03	1.063E+03	1.063E+03	1.063E+03

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bulk gas transport properties at time = 1.25000E+03 s

i, j	Reynolds number	axial velocities (m/s)	radial velocities (m/s)	boundary layer	diffusive thickness	boundary layer	diffusive thickness	density (kg/m**3)	conductivity (W/mK)	viscosity (Pa-s)
1, 1	5.399E+03	1.560E+00	1.059E+00	8.012E-03	8.012E-03	3.852E-03	3.852E-03	4.330E-01	6.435E-02	2.744E-05
2, 1	3.988E+03	1.497E+00	.	2.698E-03	2.698E-03	3.552E-03	3.552E-03	4.330E-01	6.435E-02	2.744E-05
1, 2	8.936E+03	1.560E+00	.	5.344E-03	5.344E-03	3.839E-03	3.839E-03	4.330E-01	6.435E-02	2.744E-05
2, 2	6.513E+03	1.497E+00	.	2.866E-03	2.866E-03	3.539E-03	3.539E-03	4.330E-01	6.435E-02	2.744E-05
1, 3	3.393E+04	1.512E+00	.	7.074E-03	7.074E-03	1.000E-04	1.000E-04	4.330E-01	6.435E-02	2.744E-05
2, 3	2.374E+04	1.453E+00	.	4.035E-03	4.035E-03	1.000E-04	1.000E-04	4.330E-01	6.435E-02	2.744E-05
1, 4	3.340E+04	1.512E+00	.	7.150E-03	7.150E-03	1.000E-04	1.000E-04	4.330E-01	6.435E-02	2.744E-05
2, 4	2.338E+04	1.453E+00	.	4.267E-03	4.267E-03	1.000E-04	1.000E-04	4.330E-01	6.435E-02	2.744E-05
1, 5	3.340E+04	1.512E+00	.	7.137E-03	7.137E-03	1.000E-04	1.000E-04	4.330E-01	6.435E-02	2.744E-05
2, 5	2.338E+04	1.453E+00	.	4.402E-03	4.402E-03	1.000E-04	1.000E-04	4.330E-01	6.435E-02	2.744E-05
1, 6	1.508E+05	1.210E+01	-1.059E+00	2.134E-03	2.134E-03	1.000E-04	1.000E-04	4.330E-01	6.435E-02	2.744E-05
2, 6	1.447E+04	.	.	4.830E-03	4.830E-03	1.000E-04	1.000E-04	4.330E-01	6.435E-02	2.744E-05

Description of VICTORIA Output

7.1.6 Species Mass Concentrations

The next section contains the mass concentrations of each species, as shown on the following pages for node $i=1$, $j=1$. The output file lists these data for each node defined in the problem; however, for brevity, only the data for the first node are included here.

Mass concentrations are given for each condensed- and vapor-phase species and for each subregion of the node. Since there are two fuel subnodes in this example, data are given separately for these two subnodes. The data are further categorized as mass concentrations within the grains and within the pores. Only elemental species are allowed to exist within the grains, so all other concentrations are zero, as indicated by a dot (.).

Following the data for the fuel, the mass concentrations are given for each of the other subregions described in Chapter 3: the fuel/clad gap, the cladding; the boundary layer or film on the exterior surface of the fuel rods; the boundary layer on the exterior surface of the control rods; the bulk gas, including gases and aerosols; and the boundary layer adjacent to structural surfaces. The final column of data gives the total quantity of each species, summed over the subregions. These values are expressed as masses rather than as concentrations. The final row of data contains a calculated total gas pressure in each subregion where vapors exist. This total pressure is calculated by summing the partial pressures of all of the vapor-phase species. In this example, the total gas pressures in some regions are calculated to be higher than the specified input value of $1.5 \cdot 10^5$ Pa, as shown in the temperature and pressure data above. However, the calculated value in the bulk gas is very close to the input value.

Two lines of output provide information on chemisorption of cesium and tellurium. No stainless steel structures are defined in this node, so the chemisorption of cesium onto stainless steel structures is determined to be zero. A very small amount of tellurium is calculated to be chemisorbed onto the Zircaloy cladding.

Description of VICTORIA Output

species densities (kg/m**3) at i = 1 j = 1 time = 1.25000E+03 s

species	grains	1	pores	1	grains	2	pores	2	gap	clad	1	film	control	bulk gas	aerosol
CsIc	.	3.948E-04	.	1.588E-03	5.808E-04	.	1.047E-09	8.617E-10	3.694E-03	.	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
CsIg	.	7.908E-09	.	2.500E-08	4.854E-09	.	3.771E-05	3.481E-04	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
CsOhc	.	4.633E-07	.	3.771E-05	3.481E-04	.	3.370E-08	2.040E-07	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
CsOHg	.	4.863E-10	.	3.370E-08	2.040E-07	.	5.327E-09	7.984E-12	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
CsHg	.	5.954E-09	.	5.327E-09	7.984E-12	.	4.373E-20	6.946E-21	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
Cs2Og	.	7.233E-22	.	4.373E-20	6.946E-21	.	4.066E-15	2.727E-13	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
Cs2O2H2g	.	6.720E-19	.	4.066E-15	2.727E-13	.	2.485E-07	4.620E-10	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
Csc	3.513E-94	2.560E-07	3.294E-86	2.485E-07	4.620E-10	.	7.496E-18	2.489E-18	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
Cs2Oc	.	9.334E-20	.	7.496E-18	2.489E-18	.	4.390E-19	1.722E-11	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
Cs2UO4c	.	2.683E-22	.	4.390E-19	1.722E-11	.	3.700E-28	4.729E-13	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
Cs2U2O7c	.	1.817E-32	.	3.700E-28	4.729E-13	.	2.330E-04	1.791E-07	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
Cs2MoO4c	.	6.203E-12	.	2.330E-04	1.791E-07	.	1.842E-11	7.967E-17	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
BaOHg	.	2.543E-11	.	1.842E-11	7.967E-17	.	2.839E-08	6.189E-10	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
BaO2H2g	.	4.651E-10	.	2.839E-08	6.189E-10	.	1.703E+00	9.765E-02	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
BaO2H2c	.	1.929E-02	.	1.703E+00	9.765E-02	.	4.030E-14	1.453E-18	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
BaOg	.	4.030E-14	.	2.553E-14	1.453E-18	.	1.038E+02	2.768E-02	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
BaOc	.	9.082E+01	.	1.038E+02	2.768E-02	.	9.912E-16	1.087E-22	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
BaIg	.	3.284E-14	.	9.912E-16	1.087E-22	.	1.641E-12	3.509E-18	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
BaI2g	.	1.641E-12	.	1.925E-13	3.509E-18	.	8.097E-04	6.142E-09	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
BaI2c	.	8.097E-04	.	1.348E-04	6.142E-09	.	5.227E-16	4.297E-25	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
BaHg	.	6.187E-14	.	5.227E-16	4.297E-25	.	4.848E-10	6.918E-19	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
Bac	1.941E-94	4.649E-08	1.820E-86	4.848E-10	6.918E-19	.	3.080E-01	4.968E-10	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
BaTec	.	8.139E+01	.	3.080E-01	4.968E-10	.	4.612E-05	1.063E+00	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
BaUO4c	.	2.228E-06	.	4.612E-05	1.063E+00	.	1.491E+02	4.924E-05	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
BaMoO4c	.	3.531E-04	.	1.491E+02	4.924E-05	.	3.249E-12	1.424E-10	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
Ig	2.587E-95	1.393E-12	2.426E-87	3.249E-12	1.424E-10	.	2.926E-11	2.413E-11	4.854E-09	1.047E-09	.	8.617E-10	2.179E-11	6.337E-13	1.074E-04
Test Problem (NEB)															
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Test Problem (NEB)

species densities (kg/m**3) at i = 1 j = 1 time = 1.25000E+03 s

species	grains	1	pores	1	grains	2	pores	2	gap	clad	1	film	control	bulk gas	aerosol
I2g	.	4.011E-22	.	2.676E-21	8.750E-18	.	2.092E-18	1.761E-18	5.222E-19	2.419E-21	1.074E-04	1.074E-04	1.074E-04	1.074E-04	1.074E-04
HIg	.	1.256E-10	.	3.270E-10	1.022E-09	.	1.999E-10	1.625E-10	7.227E-12	2.556E-13	1.074E-04	1.074E-04	1.074E-04	1.074E-04	1.074E-04
Hg	.	1.126E-10	.	8.275E-11	1.985E-12	.	3.098E-13	1.912E-13	6.702E-18	3.482E-18	1.074E-04	1.074E-04	1.074E-04	1.074E-04	1.074E-04
H2g	.	4.562E-02	.	4.539E-02	1.285E-04	.	1.270E-04	9.944E-05	5.989E-08	1.617E-08	1.074E-04	1.074E-04	1.074E-04	1.074E-04	1.074E-04
H2Og	.	3.911E-05	.	2.691E-03	4.273E-01	.	4.274E-01	4.278E-01	4.330E-01	4.330E-01	1.074E-04	1.074E-04	1.074E-04	1.074E-04	1.074E-04
SrOHg	.	2.940E-16	.	4.742E-15	4.421E-18	.	1.127E-17	9.379E-18	9.847E-32	4.731E-44	1.074E-04	1.074E-04	1.074E-04	1.074E-04	1.074E-04
SrO2H2c	.	4.355E-05	.	9.030E-02	1.281E+00	.	1.517E-12	1.271E-12	1.198E-04	1.553E-33	1.033E-17	1.033E-17	1.033E-17	1.033E-17	1.033E-17
SrO2H2g	.	1.139E-15	.	1.528E-12	6.928E-12	.	1.742E+00	1.742E+00	1.117E-05	1.022E-51	1.033E-17	1.033E-17	1.033E-17	1.033E-17	1.033E-17
SrOc	.	8.84E-01	.	2.446E+01	1.742E+00	.	9.724E-25	8.227E-25	1.106E-39	5.191E-50	1.033E-17	1.033E-17	1.033E-17	1.033E-17	1.033E-17
SrOg	.	1.792E-23	.	2.233E-22	1.982E-24	.	3.889E-22	2.991E-20	3.055E-36	1.979E-44	9.227E-32	9.227E-32	9.227E-32	9.227E-32	9.227E-32
SrIg	.	2.111E-17	.	1.479E-17	3.889E-22	.	1.893E-19	1.141E-19	1.712E-29	1.724E-54	5.146E-47	5.146E-47	5.146E-47	5.146E-47	5.146E-47
SrI2g	.	1.809E-17	.	4.753E-17	1.893E-19	.	6.063E-11	2.376E-20	7.980E-17	2.061E-34	5.881E-33	5.881E-33	5.881E-33	5.881E-33	5.881E-33
SrI2c	.	1.798E-09	.	6.527E-09	6.063E-11	.	2.721E-20	2.376E-20	7.980E-17	2.061E-34	5.881E-33	5.881E-33	5.881E-33	5.881E-33	5.881E-33
Srg	.	4.903E-17	.	9.688E-18	1.949E-24	.	1.787E-19	1.787E-19	4.185E-09	8.284E-08	1.792E-27	1.792E-27	1.792E-27	1.792E-27	1.792E-27
Src	1.256E-94	2.199E-12	1.178E-86	5.295E-13	1.787E-19	.	2.337E+00	2.337E+00	8.284E-08	1.724E-54	5.146E-47	5.146E-47	5.146E-47	5.146E-47	5.146E-47
SrUO4c	.	8.463E-10	.	4.111E-07	2.337E+00	.	2.516E-03	2.516E-03	8.284E-08	1.724E-54	5.146E-47	5.146E-47	5.146E-47	5.146E-47	5.146E-47
SrMoO4c	.	2.758E-06	.	2.825E+01	2.516E-03	.	2.516E-03	2.516E-03	8.284E-08	1.724E-54	5.146E-47	5.146E-47	5.146E-47	5.146E-47	5.146E-47
Zrc	2.079E+01	.	2.079E+01	.	2.079E+01	.	2.079E+01	2.079E+01	1.723E-17	1.165E-34	1.792E-27	1.792E-27	1.792E-27	1.792E-27	1.792E-27
Snc	6.381E-96	2.372E+00	5.984E-88	1.277E+00	1.249E-06	.	6.943E-15	5.792E-15	1.723E-17	1.165E-34	1.792E-27	1.792E-27	1.792E-27	1.792E-27	1.792E-27
Sng	.	8.636E-12	.	3.097E-12	1.048E-18	.	6.943E-15	5.792E-15	1.723E-17	1.165E-34	1.792E-27	1.792E-27	1.792E-27	1.792E-27	1.792E-27

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Description of VICTORIA Output

species	grains	1	pores	2	grains	2	pores	2	gap	clad	1	film	control	bulk gas	aerosol
SnOg	.	2.192E-13	.	5.786E-12	1.292E-13	4.303E-14	3.643E-14	1.843E-25	7.102E-35						
SnOc	.	6.607E-05	.	2.604E-03	1.657E-04	.	.	2.762E-11						1.064E-20	
SnO2c	.	5.166E-09	.	1.483E-05	6.056E-02	.	.	1.028E-04						1.467E-13	
SnO2g	.	7.490E-28	.	1.058E-24	6.788E-22	1.592E-22	1.355E-22	1.562E-33	2.230E-42					2.230E-42	
SnI2g	.	1.246E-19	.	5.001E-19	2.135E-21	1.765E-21	1.487E-21	4.162E-32	2.005E-44					5.430E-43	
SnI2c	.	1.944E-18	.	7.881E-18	3.464E-20	.	.	1.127E-30						1.308E-46	
SnTeq	.	1.133E-05	.	1.235E-06	2.976E-13	2.687E-09	2.199E-09	7.026E-34	1.308E-46					7.885E-39	
SnTeq	.	6.036E-01	.	8.124E-02	3.402E-08	.	.	4.235E-26						3.678E-58	
SnH4g	.	3.300E-15	.	1.422E-15	6.413E-27	3.304E-18	2.784E-18	4.852E-47	5.643E-23					2.964E-13	
Teg	5.431E-95	9.214E-08	.	1.686E-08	3.190E-09	7.030E-10	5.818E-10	1.656E-10							
Te2g	.	5.210E-07	.	3.610E-02	1.296E-02	3.783E-14	4.254E-10	7.348E-27	2.354E-32					2.640E-16	
TeOg	.	8.929E-17	.	2.501E-08	2.294E-09	5.197E-10	4.254E-10	7.348E-27	2.354E-32					1.202E-23	
TeO2g	.	1.917E-27	.	9.690E-16	6.886E-12	1.581E-12	1.340E-12	1.812E-21	5.009E-26					1.379E-36	
TeO2c	.	7.094E-22	.	1.225E-24	3.207E-16	1.304E-16	1.218E-16	2.039E-24	5.009E-26					5.036E-26	
Te2O2g	.	1.328E-27	.	6.045E-19	3.369E-10	.	.	1.075E-14						.	
H2Teq	.	1.541E-06	.	2.186E-25	2.650E-17	6.618E-18	5.712E-18	3.138E-32	1.379E-36						
UO2c	.	5.490E-06	.	3.271E-07	2.618E-10	8.574E-10	7.276E-10	1.042E-22	5.036E-26						
UO2g	.	2.883E-29	.	1.270E-06	1.419E-03	.	.	1.347E-11							
Uc	8.994E+03	2.807E-24	.	2.907E-30	3.716E-28	.	.	1.470E-46							
Ug	.	2.340E-44	.	5.981E-29	2.503E-36	.	.	2.969E-61							
U4O9c	.	9.117E-37	.	2.574E-49	1.915E-57	.	.	1.153E-90							
U3O8c	.	1.459E-39	.	1.583E-37	9.810E-21	.	.	4.511E-51							
UO3c	.	1.748E-16	.	6.610E-38	1.442E-19	.	.	3.146E-40							
Krg	4.880E-95	1.337E-13	.	2.422E-15	1.042E-07	.	.	3.500E-14							
Xeg	6.706E-94	1.409E-12	.	1.268E-13	8.704E-14	8.705E-14	8.698E-14	8.378E-14	8.650E-14						
O2g	.	3.027E-28	.	1.336E-12	9.150E-13	9.151E-13	9.143E-13	9.371E-13	9.083E-13						
	.		.	7.318E-25	3.876E-16	2.562E-12	2.678E-12	5.604E-18	7.688E-17						

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Test Problem (NEB)

species densities (kg/m**3) at i = 1 j = 1 time = 1.25000E+03 s

species	grains	1	pores	2	grains	2	pores	2	gap	clad	1	film	control	bulk gas	aerosol
Og	1.221E+03	2.948E-24	1.024E-22	9.511E-19	1.018E-15	1.063E-15	5.229E-24	1.937E-23	4.782E-43						
Moc	4.039E-94	4.328E+02	3.732E+02	1.336E-15	.	.	3.165E-28	1.120E-82	1.877E-71						
Moq	.	4.061E-25	1.428E-25	4.919E-44	.	.	7.411E-68	3.354E-57	1.842E-13						
MoOg	.	1.471E-25	3.878E-24	9.250E-38	.	.	1.842E-13	9.218E-44	1.911E-57						
MoO2c	.	5.933E-05	2.757E-01	4.245E-09	1.002E-23	8.206E-24	9.739E-16	3.677E-46	1.048E-27						
MoO2g	.	2.283E-24	4.914E-21	1.013E-29	8.398E-23	7.207E-23	4.789E-33	1.399E-40	5.400E-13						
MoO3c	.	2.230E-14	1.013E-29	2.989E-12	3.365E-13	3.171E-13	2.323E+02	3.912E-05	3.783E-37						
MoO3g	.	1.981E-25	3.362E-20	5.475E-24	4.049E-16	3.266E-16	3.363E-23	2.807E-33	1.372E-29						
Agg	.	5.804E-13	8.886E-13	7.574E-13	8.584E-03	.	2.270E-15	8.828E-20	1.307E-24						
Agc	.	1.739E-03	3.847E-03	8.584E-03	2.057E-15	4.049E-16	3.912E-05	8.828E-20	6.774E-41						
AgTeq	.	1.703E-14	6.261E-15	2.770E-08	2.733E-20	1.118E-20	3.912E-05	8.828E-20	3.174E-37						
Ag2Tec	.	2.062E-08	3.470E-18	2.733E-20	2.733E-20	1.118E-20	3.912E-05	8.828E-20	8.411E-41						
Cdg	.	3.665E-18	2.733E-20	2.733E-20	2.733E-20	1.118E-20	3.912E-05	8.828E-20	8.015E-58						
Cdc	.	2.996E-16	3.470E-18	2.733E-20	2.733E-20	1.118E-20	3.912E-05	8.828E-20	4.778E-50						
CdOc	.	4.867E-22	3.669E-20	2.345E-17	2.345E-17	.	2.270E-15	8.828E-20							
CdOg	.	4.761E-32	2.299E-30	4.587E-28	4.587E-28	.	2.270E-15	8.828E-20							
CdTeq	.	9.268E-15	2.782E-15	1.747E-17	1.747E-17	.	1.177E-31	6.774E-41							
CdTeq	.	1.661E-25	3.197E-26	6.281E-29	6.281E-29	.	1.177E-31	6.774E-41							
Ing	.	1.371E-37	7.610E-39	3.747E-42	3.747E-42	.	1.141E-24	2.687E-54							
Inc	.	4.087E-29	3.124E-30	3.547E-33	3.547E-33	.	1.656E-53	8.450E-54							
In2O3c	.	5.636E-70	1.434E-66	6.704E-58	6.704E-58	.	1.648E-40	2.687E-54							
InTeq	.	7.197E-29	1.522E-30	9.605E-34	9.605E-34	.	5.230E-47	1.929E-65							
InTeq	.	2.686E-38	3.688E-40	7.551E-44	7.551E-44	.	2.112E-62	1.929E-65							
InOHg	.	5.131E-258	5.133E-260	1.386E-266	1.386E-266	.	.	.							

Description of VICTORIA Output

Rug	1.871E-24	7.844E-25	2.752E-33	.	.	.	1.483E-48	.	.
Ruc	3.117E+02	3.196E+02	1.159E-05	.	.	.	9.343E-10	.	.
RuO2c	1.027E-18	3.789E-15	2.054E-13	.	.	.	2.530E-14	.	.
RuO3g	6.456E-40	8.708E-35	5.016E-29	.	.	.	1.353E-34	.	.
RuO4g	1.360E-52	1.034E-45	1.954E-35	.	.	.	3.314E-40	.	.
Sbg	3.727E-09	1.458E-09	4.197E-12	4.047E-12	3.351E-12	5.686E-21	1.988E-28	2.031E-15	
Sbc	1.060E+00	5.718E-01	3.810E-03	.	.	.	5.808E-08	3.420E-41	
Sb2g	1.092E+08	2.571E-09	6.550E-14	5.414E-12	4.431E-12	2.798E-26	9.604E-73	1.129E-19	
Sb4g	8.631E-13	6.875E-14	1.148E-22	1.735E-16	1.467E-16	6.428E-43	8.106E-37	1.413E-70	
Sb2O3c	2.625E-20	2.266E-15	1.338E-05	.	.	.	2.015E-47	.	
SbTe2g	1.057E-07	1.105E-08	1.619E-11	2.736E-11	2.239E-11	1.295E-26	.	.	
Sb2Te3c	2.326E-09	1.095E-11	4.169E-17	.	.	.	7.786E-50	.	
Rug	3.895E-20	1.237E-22	2.290E-31	1.357E-24	1.226E-24	7.786E-50	.	.	
Ruc	5.457E-15	2.137E-17	6.833E-26	.	.	.	1.091E-41	.	
EuOg	1.460E-24	3.078E-25	2.868E-29	.	.	.	6.618E-45	.	
EuOc	3.166E-05	1.339E-05	7.695E-09	.	.	.	9.870E-16	.	
Eu2O3c	3.983E-01	7.892E+00	4.990E-01	.	.	.	1.502E-05	.	
EuTe2g	2.362E-19	1.915E-22	1.600E-31	4.032E-24	3.311E-24	8.677E-57	.	.	
H2MoO4g	4.845E-10	6.941E-12	6.580E-25	2.433E-14	2.058E-14	9.855E-64	3.416E-89	6.194E-34	
Heg	4.491E-22	7.321E-15	4.537E-16	1.130E-16	9.414E-17	8.068E-21	5.725E-15	6.936E-24	
CsOg	8.038E-15	7.728E-15	5.741E-15	5.741E-15	5.737E-15	5.782E-15	6.936E-24	4.978E-35	
Cs2g	3.823E-22	1.816E-20	7.736E-19	1.152E-18	1.165E-18	4.383E-24	7.214E-21	2.727E-34	
Cs2g	3.326E-18	2.839E-18	7.551E-24	8.166E-21	7.214E-21	2.727E-34	4.978E-35	.	

Test Problem (NEB)
species densities (kg/m**3) at i = 1 j = 1 time = 1.25000E+03 s
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species	grains	1 pores	1 grains	2 pores	2 gap	clad	1 film	control	bulk gas	aerosol
CsHg	.	4.167E-12	.	3.520E-12	2.437E-16	9.074E-15	7.830E-15	2.748E-24	6.099E-25	.
Cs2U4O12c	.	2.058E-57	.	1.789E-52	2.347E-26	.	.	2.222E-49	.	3.400E-22
Cs2Tec	.	1.739E-03	.	6.822E-04	3.838E-09	.	.	1.041E-18	.	5.104E-15
Cs2TeO3c	.	1.502E-25	.	1.633E-20	1.025E-11	.	.	3.074E-13	.	1.841E-29
Cs2Te2O5c	.	2.763E-47	.	2.880E-39	1.376E-21	.	.	4.515E-26	.	3.178E-61
Cs2Te4O9c	.	1.355E-92	.	1.192E-78	2.643E-43	.	.	1.292E-54	.	2.600E-19
Cs2TeO4c	.	8.436E-38	.	5.248E-31	1.133E-17	.	.	4.228E-18	.	7.227E-80
Cs2Te4O12c	.	1.396-134	.	2.288-115	1.991E-66	.	.	5.781E-75	.	.
Cs2O2g	.	9.938E-63	.	1.698E-59	1.481E-56	.	.	9.672E-71	2.422E-70	
Cs2I2g	.	3.240E-14	.	4.613E-13	4.459E-14	1.248E-14	1.080E-14	1.062E-13	8.975E-17	
Cs2WoO4g	.	1.339E-21	.	3.698E-14	1.290E-17	7.612E-17	6.200E-17	1.885E-20	9.786E-34	
IOg	.	5.673E-32	.	5.878E-30	4.553E-24	.	.	4.312E-28	1.087E-28	
HOg	.	5.565E-16	.	2.597E-14	2.795E-11	6.078E-12	5.113E-12	1.855E-14	3.571E-14	
HIog	.	5.921E-22	.	9.027E-20	1.035E-14	2.620E-15	2.269E-15	3.112E-15	4.076E-16	
BaHg	.	9.553E-17	.	7.614E-19	2.885E-29	3.190E-21	2.648E-21	3.295E-48	1.483E-58	
Ba2Og	.	2.394E-18	.	1.935E-20	2.661E-33	7.695E-23	6.321E-23	5.537E-57	1.539E-76	
BaH2c	.	1.577E-06	.	2.154E-08	1.784E-19	.	.	2.717E-33	6.354E-44	
Ba2g	.	1.722E-29	.	1.311E-33	1.060E-51	.	.	8.739E-84	6.556-104	
Ba2O2g	.	7.937E-33	.	3.517E-33	1.497E-41	.	.	2.322E-64	2.390E-83	
BaMoO4g	.	3.802E-22	.	8.311E-17	4.989E-24	1.755E-19	1.452E-19	6.690E-36	1.648E-58	
SrH2c	.	2.013E-10	.	6.321E-11	1.225E-19	.	.	1.723E-34	1.161E-47	
Sr2g	.	3.286E-35	.	1.384E-36	6.900E-50	.	.	1.758E-83	1.095-108	
SrOg	.	8.208-229	.	5.816-230	1.372-239	
SnH2O2g	.	2.914-250	.	9.931-250	2.734-256	
Sn2g	.	1.746E-17	.	3.063E-18	7.972E-31	6.502E-21	5.321E-21	1.787E-58	1.934E-78	
SnTe2g	.	5.278E-21	.	1.031E-22	4.509E-30	.	.	1.792E-61	5.973E-77	
TeO3H2g	.	3.416E-31	.	1.834E-26	1.302E-15	3.213E-16	2.767E-16	8.598E-21	2.112E-22	
TeI4g	.	7.995E-50	.	9.878E-49	6.048E-42	.	.	1.880E-49	7.220E-57	

Description of VICTORIA Output

species densities (kg/m**3) at i = 1 j = 1 time = 1.25000E+03 s													
species	grains	1	pores	1	grains	2	pores	2	gap	clad	1	film	control
												bulk gas	aerosol
TeO12g	.	3.587E-36	.	3.426E-34	1.666E-26	.	3.426E-34	1.666E-26	.	1.496E-24	1.497E-24	2.861E-33	8.787E-38
TeI4c	.	9.861E-52	.	1.316E-50	9.822E-44	.	1.316E-50	9.822E-44	.	.	.	2.188E-50	8.402E-58
TeH2O4c	.	1.081E-44	.	3.757E-38	1.264E-22	.	3.757E-38	1.264E-22	.	.	.	3.641E-25	3.313E-26
TeOHg	.	1.110-229	.	3.470-231	3.133-235	.	3.470-231	3.133-235	.	.	.	5.544-319	2.144-321
TeH2O2g	.	2.327-251	.	3.517-251	3.753-252	.	3.517-251	3.753-252
UH4O5c	.	1.633E-31	.	1.129E-26	1.442E-14	.	1.129E-26	1.442E-14	.	.	.	1.939E-19	.
UOg	.	2.096E-37	.	2.188E-40	2.101E-43	.	2.188E-40	2.101E-43	.	1.496E-24	1.497E-24	5.177E-69	.
UO3g	.	2.385E-32	.	1.773E-31	1.518E-24	.	1.773E-31	1.518E-24	.	.	.	2.315E-38	.
UOHg	.	7.870-252	.	2.204-257	2.215-268	.	2.204-257	2.215-268
UH2O2g	.	7.756-273	.	1.043-276	1.219-284	.	1.043-276	1.219-284
MoI4c	.	5.514E-40	.	3.190E-38	3.622E-48	.	3.190E-38	3.622E-48	.	.	.	1.689E-57	5.475E-77
MoI3c	.	1.245E-27	.	2.673E-26	4.733E-38	.	2.673E-26	4.733E-38	.	.	.	2.005E-47	9.546E-66
MoI2c	.	1.564E-17	.	1.139E-16	2.497E-30	.	1.139E-16	2.497E-30	.	.	.	7.596E-41	5.315E-58
Mo2g	.	1.266E-35	.	2.824E-36	1.577E-72	.	2.824E-36	1.577E-72	.	.	.	1.855-112	4.233-142
Mo2O6g	.	3.923E-38	.	2.043E-27	2.586E-34	.	2.043E-27	2.586E-34	.	.	.	2.439E-44	1.438E-70
MoOHg	.	8.500-225	.	9.582-226	8.135-247	.	9.582-226	8.135-247
MoH2O2g	.	1.109-246	.	6.064-246	6.140-264	.	6.064-246	6.140-264
In2Og	.	1.928E-24	.	1.831E-24	1.253E-24	.	1.831E-24	1.253E-24	.	1.252E-24	1.252E-24	1.288E-24	1.243E-24
MoI9	.	3.279E-28	.	4.008E-28	1.730E-44	.	4.008E-28	1.730E-44	.	.	.	7.907E-65	8.130E-81
Test Problem (NEB)													
species densities (kg/m**3) at i = 1 j = 1 time = 1.25000E+03 s													
species	grains	1	pores	1	grains	2	pores	2	gap	clad	1	film	control
												bulk gas	aerosol
MoI2g	.	1.119E-28	.	5.112E-28	3.324E-42	.	5.112E-28	3.324E-42	.	.	.	2.106E-58	1.473E-75
MoI3g	.	9.250E-38	.	1.279E-36	7.217E-49	.	1.279E-36	7.217E-49	.	.	.	1.343E-63	6.397E-82
MoO212g	.	1.267E-28	.	3.875E-24	1.908E-28	.	3.875E-24	1.908E-28	.	.	.	1.063E-33	1.020E-49
Mo3O9g	.	1.023E-50	.	1.530E-34	1.254E-44	.	1.530E-34	1.254E-44	.	.	.	7.801E-57	3.531E-96
Mo4O12g	.	2.882E-66	.	1.175E-44	5.448E-58	.	1.175E-44	5.448E-58	.	.	.	4.789E-73	1.664-125
Mo5O15g	.	5.689E-83	.	6.166E-56	1.513E-72	.	6.166E-56	1.513E-72	.	.	.	8.955E-91	2.389-156
MoI4g	.	2.999E-48	.	1.210E-46	5.378E-57	.	1.210E-46	5.378E-57	.	.	.	1.033E-70	3.346E-90
AgIc	.	1.704E-11	.	1.081E-10	1.814E-08	.	1.081E-10	1.814E-08	.	.	.	8.229E-03	4.476E-19
AgIg	.	8.312E-17	.	4.215E-16	3.937E-14	.	4.215E-16	3.937E-14	.	9.697E-15	8.352E-15	1.280E-27	1.235-321
AgOHg	.	8.629-232	.	2.525-232	1.375-235	.	2.525-232	1.375-235	.	.	.	3.433-307	.
AgH2O2g	.	1.281-252	.	1.802-251	1.142-251	.	1.802-251	1.142-251
CdOHg	.	5.826-245	.	8.219-246	2.160-251	.	8.219-246	2.160-251
CdH2O2g	.	1.525-266	.	1.044-265	3.273-268	.	1.044-265	3.273-268
CdIg	.	1.071E-30	.	2.574E-30	1.109E-30	.	2.574E-30	1.109E-30	.	.	.	1.227E-34	1.298E-45
CdI2c	.	2.769E-31	.	2.730E-30	2.263E-28	.	2.730E-30	2.263E-28	.	.	.	5.673E-27	4.084E-39
CdI2g	.	3.816E-33	.	3.291E-32	1.915E-30	.	3.291E-32	1.915E-30	.	.	.	7.243E-31	5.214E-43
InIc	.	7.782E-35	.	1.863E-35	2.017E-36	.	1.863E-35	2.017E-36	.	.	.	1.264E-41	4.389E-43
InIg	.	7.680E-37	.	1.605E-37	1.210E-38	.	1.605E-37	1.210E-38	.	.	.	7.268E-46	2.525E-47
InH2O2g	.	9.942-279	.	4.756-279	1.476-282	.	4.756-279	1.476-282
Ru3Uc	.	1.543E-14	.	4.571E-19	1.782E-48	.	4.571E-19	1.782E-48	.	.	.	3.087E-82	.
RuTe2c	.	3.017E+01	.	2.244E+00	2.208E-08	.	2.244E+00	2.208E-08	.	.	.	1.455E-24	.
RuO2g	.	1.273E-32	.	2.717E-29	3.560E-28	.	2.717E-29	3.560E-28	.	.	.	1.322E-35	.
RuOg	.	4.248E-27	.	1.322E-25	3.155E-29	.	1.322E-25	3.155E-29	.	.	.	6.012E-40	.
RuOHg	.	8.307-225	.	1.103-225	9.250-237	.	1.103-225	9.250-237	.	.	.	4.310-317	.
RuH2O2g	.	1.491-246	.	9.586-246	9.543-254	.	9.586-246	9.543-254
SbOHg	.	8.052-229	.	5.839-230	9.911-236	.	5.839-230	9.911-236	.	.	.	2.367-316	.
SbH2O2g	.	6.745-250	.	2.345-249	4.610-252	.	2.345-249	4.610-252
SbH3g	.	1.529E-10	.	6.974E-11	4.614E-17	.	6.974E-11	4.614E-17	.	1.564E-13	1.306E-13	8.041E-29	3.944E-37
EuOHg	.	3.110-244	.	1.602-247	1.234-259	.	1.602-247	1.234-259
EuH2O2g	.	1.000-265	.	2.494-267	2.278-276	.	2.494-267	2.278-276
Eu2Og	.	8.135E-36	.	8.330E-39	4.403E-51	.	8.330E-39	4.403E-51	.	.	.	2.122E-79	.
Eu2O2g	.	1.237E-33	.	1.074E-34	5.435E-42	.	1.074E-34	5.435E-42	.	.	.	2.356E-64	.

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Description of VICTORIA Output

press. (Pa) 1.980E+05 1.959E+05 2.020E+05 1.979E+05 1.980E+05 2.000E+05 1.500E+05

Cesium Hydroxide chemisorption (structures) 0.000E+00 (kg)

Tellurium chemisorption (Zircaloy cladding) 3.783E-14 (kg)

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species densities (kg/m**3) at i = 1 j = 1 time = 1.25000E+03 s

species	structure	total	(kg)
CsIc	5.448E-03	1.367E-04	
CsIg	3.214E-11	1.366E-12	
CsOHC	4.383E-03	1.256E-04	
CsOHg	2.119E-08	6.252E-10	
Csg	4.079E-16	3.590E-14	
Cs20g	1.274E-24	8.351E-25	
Cs202H2g	2.428E-12	2.553E-14	
Csc	2.772E-13	1.334E-12	
Cs20c	1.125E-18	1.188E-20	
Cs2U04c	2.623E-13	2.817E-15	
Cs2U207c	1.435E-22	4.968E-18	
Cs2Mo04c	9.268E-07	1.031E-08	
BaOHg	3.723E-29	1.210E-16	
Ba02H2g	6.802E-18	1.997E-13	
Ba02H2c	5.681E-05	8.375E-06	
BaOg	8.686E-31	1.743E-19	
BaOc	5.284E-07	5.313E-04	
BaIg	2.616E-37	4.826E-20	
BaI2g	1.764E-29	3.095E-18	
BaI2c	8.814E-16	1.603E-09	
Bag	5.330E-42	8.487E-20	
Bac	4.299E-33	6.329E-14	
BaTec	4.082E-22	1.087E-04	
BaU04c	1.391E-08	1.116E-05	
BaMo04c	5.736E-12	5.904E-04	
Ig	1.181E-13	1.092E-13	
I2g	2.150E-21	2.826E-21	
Hg	3.175E-13	2.855E-13	
Hg	4.589E-18	5.917E-16	
H2g	2.808E-08	3.002E-07	
H20g	4.329E-01	3.332E-01	
SrOHg	7.619E-32	2.355E-20	
Sr02H2c	1.353E-04	1.519E-05	
Sr02H2g	1.897E-21	6.658E-16	
SrOc	1.263E-05	1.165E-04	
SrOg	1.250E-39	1.309E-27	
SrIg	1.039E-37	9.773E-23	
SrI2g	3.736E-32	2.670E-22	
SrI2c	1.741E-19	2.886E-14	
Srg	3.661E-42	1.140E-22	
Src	1.092E-34	5.001E-18	
SrU04c	4.989E-09	2.456E-05	
SrMo04c	1.276E-10	1.119E-04	

Zrc 2.635E-03
Snc 4.126E-18
Sng 2.791E-35
1

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Test Problem (NEB)

species	structure	total (kg)
SnOg	9.412E-26	4.137E-17
SnOc	1.410E-11	1.214E-08
SnO2c	1.119E-04	1.774E-06
SnO2g	1.701E-33	6.962E-26
SnI2g	4.104E-35	2.854E-24
SnI2c	1.111E-33	3.414E-23
SnTeg	6.436E-30	2.087E-11
SnTec	3.879E-22	1.119E-06
SnH4g	2.553E-48	1.127E-20
Teg	1.206E-15	4.910E-13
Tec	6.335E-06	5.468E-07
Te2g	1.075E-17	1.008E-12
TeOg	1.478E-16	6.919E-16
TeO2g	3.548E-19	6.255E-20
TeO2c	1.870E-09	1.879E-11
Te2O2g	2.088E-22	2.910E-21
H2Teg	1.869E-18	3.669E-12
UO2c	6.666E-12	1.492E-08
UO2g	7.273E-47	3.953E-33
Uc	3.230E-62	1.140E+00
Ug	1.254E-91	3.089E-50
U4O9c	5.759E-52	1.031E-25
U3O8c	1.731E-40	1.515E-24
UO3c	3.692E-14	1.095E-12
Krg	8.783E-14	6.658E-14
Xeg	9.251E-13	6.992E-13
O2g	2.548E-17	1.268E-15
Og	1.115E-23	1.541E-01
Moc	4.449E-32	2.050E-03
Mog	1.042E-71	1.102E-30
MoOg	1.005E-60	1.555E-29
MoO2c	1.177E-16	1.092E-06
MoO2g	5.891E-47	2.327E-26
MoO3c	1.327E-18	2.323E-14
MoO3g	6.526E-36	1.664E-25
Agg	1.311E-17	2.121E-16
Agc	6.752E-03	2.843E-02
AgTeg	3.739E-23	2.204E-19
Ag2Tec	1.264E-09	4.790E-09
Cdg	8.470E-24	2.414E-23
Cdc	4.140E-20	2.130E-21
CdOc	2.270E-15	2.309E-17
CdOg	1.177E-31	6.025E-33
CdTec	2.047E-20	2.365E-20
CdTeg	1.733E-37	3.465E-31
Ing	1.125E-53	2.112E-43
Inc	1.120E-40	6.637E-35
1		

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Description of VICTORIA Output

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Test Problem (NEB)

species	structure	total (kg)
In203c	2.710E-58	6.110E-58
InTec	1.359E-42	1.011E-34
InTeg	5.489E-58	3.693E-44
InOHg	.	6.977-264
Rug	1.783E-48	5.578E-30
Ruc	1.123E-09	1.678E-03
Ru02c	1.383E-13	1.395E-15
Ru03g	1.576E-33	5.428E-34
Ru04g	8.233E-39	2.881E-40
Sbg	1.981E-21	1.229E-14
Sbc	2.024E-08	3.704E-06
Sb2g	3.397E-27	2.665E-14
Sb4g	9.475E-45	1.479E-18
Sb203c	2.139E-06	2.186E-08
SbTeg	1.727E-22	1.939E-13
Sb2Te3c	1.370E-34	3.115E-15
Eug	2.657E-50	5.247E-26
Euc	3.724E-42	7.289E-21
Eu0g	4.817E-45	3.147E-30
Eu0c	7.184E-16	9.493E-11
Eu203c	1.697E-05	3.720E-05
EuTeg	1.133E-52	3.142E-25
Sn2Te2g	8.271E-56	6.766E-16
H2Mo04g	1.099E-23	7.727E-20
Heg	5.757E-15	4.406E-15
Cs0g	2.148E-22	5.435E-22
Cs2g	1.441E-31	1.895E-23
CsHg	4.324E-23	2.305E-17
Cs2U4012c	1.453E-46	2.465E-31
Cs2Tec	2.103E-11	4.998E-09
Cs2Te03c	6.023E-05	6.054E-07
Cs2Te205c	1.539E-12	1.547E-14
Cs2Te409c	1.333E-30	1.339E-32
Cs2Te04c	1.767E-09	1.776E-11
Cs2Te4012c	5.781E-50	5.810E-52
Cs202g	2.323E-67	1.557E-61
Cs212g	2.309E-13	2.410E-15
Cs2Mo04g	2.894E-20	1.756E-19
IOg	5.901E-29	1.310E-28
HOg	2.709E-14	3.003E-14
HI0g	2.915E-16	3.138E-16
BaHg	1.218E-48	1.304E-22
Ba20g	3.441E-57	3.267E-24
BaH2c	6.878E-34	2.168E-12
Ba2g	2.547E-84	2.274E-35
Ba202g	3.077E-64	2.441E-38
BaMo04g	1.050E-38	3.963E-22

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Description of VICTORIA Output

species	structure	total (kg)
SrH2c	4.282E-35	5.162E-16
Sr2g	4.938E-84	4.886E-41
SnOHg	.	1.314-234
SnH2O2g	.	4.318-255
Sn2g	1.025E-59	3.765E-23
SnTe2g	6.281E-53	7.377E-27
TeO3H2g	1.495E-15	1.517E-17
TeI4g	1.220E-49	6.353E-47
TeO12g	9.612E-31	1.847E-31
TeI4c	1.419E-50	1.032E-48
TeH2O4c	1.350E-19	1.357E-21
TeOHg	3.097-314	1.603-235
TeH2O2g	.	2.095-256
UH4O5c	2.044E-19	1.535E-19
UOg	1.201E-69	2.776E-43
UO3g	2.442E-38	6.947E-28
UOHg	.	1.039-257
UH2O2g	.	1.024-278
MoI4c	4.026E-66	1.271E-43
MoI3c	7.444E-55	1.075E-31
MoI2c	4.396E-47	4.720E-22
Mo2g	3.664-120	2.790E-41
Mo2O6g	4.529E-50	8.091E-33
MoOHg	.	1.502-230
MoH2O2g	.	2.548-251
In2Og	1.268E-24	9.568E-25
MoIg	7.132E-70	2.020E-33
MoI2g	1.219E-64	2.173E-33
MoI3g	4.989E-71	5.189E-42
MoO2I2g	2.797E-39	1.535E-29
Mo3O9g	1.974E-65	6.059E-40
Mo4O12g	1.652E-84	4.653E-50
Mo5O15g	4.208-105	2.442E-61
MoI4g	2.461E-79	4.832E-52
AgIc	5.276E-09	3.454E-07
AgIg	1.509E-17	9.925E-16
AgOHg	1.457-311	2.141-237
AgH2O2g	.	1.930-256
CdOHg	.	1.095-250
CdH2O2g	.	4.371-271
CdIg	3.692E-36	2.331E-35
CdI2c	1.095E-29	8.050E-31
CdI2g	1.399E-33	1.227E-34
InIc	5.510E-43	1.980E-40
InIg	3.169E-47	1.777E-42
InH2O2g	.	3.198-284
Ru3Uc	5.829E-83	2.037E-20

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species	structure	total (kg)
RuTe2c	2.559E-15	4.872E-05
RuO2g	7.221E-35	3.849E-33

Description of VICTORIA Output

RuOg	1.541E-39	5.295E-31
RuOHg	7.563-317	1.534-230
RuH2O2g	.	3.994-251
SbOHg	1.204-316	1.294-234
SbH2O2g	.	1.023-254
SbH3g	8.994E-30	5.385E-16
EuOHg	.	4.112-250
EuH2O2g	.	1.419-271
Eu2Og	5.272E-80	1.077E-41
Eu2O2g	1.248E-64	2.058E-39
press. (Pa)	1.500E+05	

Description of VICTORIA Output

7.1.7 Element Masses

It is often very useful to know the total masses of each element that are retained or deposited in each subregion. The tabular data shown on the following page contain this information for the node $i=1, j=1$; similar data for the other nodes are omitted for brevity. The first two columns of data in the table are for the fuel grains and pores. These data are summed over the two fuel subnodes. The subsequent columns of data contain elemental masses for each of the other subregions: the fuel/cladding gap; the fuel cladding; the boundary layer on the exterior surface of the cladding; the vapors in the bulk gas; the aerosols in the bulk gas; the boundary layer adjacent to structural surfaces; and the total of all the subregions.

The values for structural surfaces are further categorized as masses that condense directly onto the surface; those that deposit as aerosols, and those that are present as vapors within the boundary layer. The sum of these three values is given as the total. In some cases, the mass that condenses directly onto a structural surface has a negative value. This can occur when aerosols deposit onto the surface and later revaporize.

Description of VICTORIA Output

element masses (kg) at i = 1 j = 1 time = 1.250000E+03 s

element	grains	pores	gap	clad	film	control	bulk gas	aerosol	structure condensed	structure deposited
Ba	1.730E-90	8.101E-04	4.572E-06	7.081E-15	5.713E-14	4.881E-09	1.153E-27	9.734E-15	3.767E-07	8.573E-08
Cs	3.131E-90	7.572E-09	6.367E-09	1.601E-12	1.255E-11	2.448E-07	3.497E-10	1.140E-04	-2.413E-04	3.088E-04
H	.	3.261E-07	7.335E-07	2.046E-06	1.956E-05	5.874E-06	3.651E-02	5.437E-07	-1.108E-06	1.431E-06
I	2.306E-91	4.367E-09	2.981E-09	3.176E-14	2.489E-13	4.069E-07	5.227E-13	3.981E-05	-7.250E-05	9.924E-05
Mo	3.600E-90	2.284E-03	1.041E-08	3.616E-21	2.865E-20	2.067E-11	4.458E-34	5.358E-21	1.736E-09	3.628E-10
O	1.541E-01	2.326E-04	1.710E-05	1.633E-05	1.561E-04	4.699E-05	2.921E-01	8.699E-06	-1.746E-05	2.298E-05
Ru	2.665E-90	1.691E-03	1.218E-10	.	.	1.140E-13	.	.	9.149E-12	2.137E-12
Sn	5.689E-92	8.739E-06	5.026E-07	5.565E-14	4.351E-13	9.884E-09	4.750E-35	8.770E-14	7.475E-07	1.386E-07
Sr	1.120E-90	1.228E-04	3.070E-05	4.698E-17	3.759E-16	1.169E-08	8.491E-34	6.718E-17	9.084E-07	1.786E-07
Te	4.841E-91	8.817E-05	1.362E-07	1.871E-13	1.181E-12	1.775E-09	1.661E-22	2.262E-13	1.639E-07	7.476E-08
U	1.140E+00	1.124E-10	2.106E-05	5.350E-29	5.113E-28	1.071E-12	.	.	8.666E-11	1.976E-11
Zr	2.635E-03
Ag	.	1.753E-08	9.018E-08	1.466E-17	1.318E-16	2.836E-02	1.242E-27	4.098E-13	5.655E-05	1.132E-05
In	.	9.159E-30	1.231E-29	5.034E-29	4.806E-28	1.470E-28	8.819E-25	6.399E-41	-5.799E-18	5.799E-18
Cd	.	1.268E-20	3.385E-22	5.915E-25	4.589E-24	2.425E-19	2.131E-33	8.681E-25	-4.567E-07	4.567E-07
Sb	2.189E-92	3.664E-06	4.014E-08	9.874E-16	7.738E-15	1.924E-10	1.509E-28	1.541E-15	1.473E-08	3.432E-09
Eu	1.730E-91	2.745E-05	4.527E-06	1.525E-28	1.242E-27	1.584E-09	.	.	1.234E-07	2.387E-08
Kr	4.351E-91	6.786E-19	9.144E-19	3.741E-18	3.571E-17	1.084E-17	6.565E-14	.	.	.
Xe	5.978E-90	7.149E-18	9.613E-18	3.933E-17	3.754E-16	1.144E-16	6.894E-13	.	.	.
He	.	4.122E-20	6.031E-20	2.467E-19	2.355E-18	7.058E-19	4.344E-15	.	.	.

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element masses (kg) at i = 1 j = 1 time = 1.250000E+03 s

element	structure vapor	structure total	total
Ba	5.480E-20	4.625E-07	8.151E-04
Cs	1.890E-10	6.743E-05	1.816E-04
H	4.834E-04	4.837E-04	3.703E-02
I	1.633E-13	2.674E-05	6.697E-05
Mo	6.559E-23	2.099E-09	2.284E-03
O	3.867E-03	3.873E-03	4.506E-01
Ru	1.129E-35	1.129E-11	1.691E-03
Sn	8.337E-28	8.861E-07	1.014E-05
Sr	1.374E-23	1.087E-06	1.546E-04
Te	2.437E-17	2.387E-07	8.855E-05
U	2.042E-40	1.064E-10	1.140E+00
Zr	.	.	2.635E-03
Ag	2.015E-19	6.786E-05	2.843E-02
In	1.192E-26	1.192E-26	8.945E-25
Cd	8.513E-26	1.997E-17	2.022E-17
Sb	2.076E-23	1.816E-08	3.723E-06
Eu	4.380E-47	1.473E-07	3.213E-05
Kr	8.828E-16	8.828E-16	6.658E-14
Xe	9.298E-15	9.298E-15	6.992E-13
He	5.786E-17	5.786E-17	4.406E-15

Description of VICTORIA Output

7.1.8 Aerosol Densities

Aerosol density data are shown on the following pages for the node $i = 1, j = 1$; for brevity, data for the other nodes are not shown. These densities are expressed as mass of aerosol per volume of bulk gas. The data are tabulated by aerosol (condensed-phase) species and by particle mass. The particle masses listed in the table correspond to the collocation points in the finite element method used to solve for aerosol behavior, as described in Part IV of this report. Linear finite elements were chosen for this problem, so the aerosol densities interpolate linearly between the values given in the table.

The values chosen in the input data for this example cause the collocation points to be spaced by factors of 10 in mass, which corresponds to factors of the cube root of 10 in radius. The radius for each particle size is given just below the mass. The radii can evolve over the course of a calculation because the aerosol density can change. They can also depend on location within the domain, i.e., they can vary from node to node.

At the bottom of the aerosol density table is a row of values that express the total mass concentrations for each particle size. These values are the sum over the aerosol species for each particle size.

Description of VICTORIA Output

aerosol densities (kg/m**3) at i = 1 j = 1 time = 1.25000E+03 s

mass (kg)	1.0E-22	1.0E-21	1.0E-20	1.0E-19	1.0E-18	1.0E-17	1.0E-16	1.0E-15	1.0E-14	1.0E-13
radius (m)	1.8E-09	3.9E-09	8.4E-09	1.8E-08	3.9E-08	8.4E-08	1.8E-07	3.9E-07	8.4E-07	1.8E-06
CsIc	2.150E-11	7.298E-09	5.480E-07	9.311E-06	4.332E-05	4.372E-05	9.825E-06	6.443E-07	1.287E-08	7.654E-11
CsOHc	2.150E-11	7.298E-09	5.480E-07	9.311E-06	4.332E-05	4.372E-05	9.825E-06	6.443E-07	1.287E-08	7.654E-11
Csc	1.032E-21	3.502E-19	2.630E-17	4.468E-16	2.079E-15	2.098E-15	4.715E-16	3.092E-17	6.177E-19	3.673E-21
Cs2Oc	1.352E-28	4.590E-26	3.446E-24	5.856E-23	2.725E-22	2.750E-22	6.179E-23	4.052E-24	8.096E-26	4.814E-28
Cs2UO4c
Cs2U2O7c	6.275E-27	2.130E-24	1.599E-22	2.717E-21	1.264E-20	1.276E-20	2.867E-21	1.880E-22	3.757E-24	2.234E-26
Cs2MoO4c	3.171E-21	1.076E-18	8.081E-17	1.373E-15	6.389E-15	6.447E-15	1.449E-15	9.501E-17	1.898E-18	1.129E-20
BaO2H2c	2.949E-23	1.001E-20	7.514E-19	1.277E-17	5.941E-17	5.995E-17	1.347E-17	8.835E-19	1.765E-20	1.050E-22
BaOc	3.185E-32	1.081E-29	8.116E-28	1.379E-26	6.417E-26	6.475E-26	1.455E-26	9.543E-28	1.907E-29	1.134E-31
BaI2c	1.381E-49	4.687E-47	3.519E-45	5.980E-44	2.782E-43	2.808E-43	6.310E-44	4.138E-45	8.268E-47	4.916E-49
Bac	6.135E-46	2.082E-43	1.563E-41	2.656E-40	1.236E-39	1.247E-39	2.803E-40	1.838E-41	3.673E-43	2.184E-45
BaUc
BaUO4c	1.804E-38	6.121E-36	4.596E-34	7.809E-33	3.634E-32	3.667E-32	8.240E-33	5.404E-34	1.080E-35	6.419E-38
BaMoO4c	2.218E-23	7.527E-21	5.651E-19	9.602E-18	4.468E-17	4.509E-17	1.013E-17	6.644E-19	1.328E-20	7.893E-23
SrO2H2c	2.068E-24	7.021E-22	5.271E-20	8.956E-19	4.167E-18	4.205E-18	9.451E-19	6.198E-20	1.238E-21	7.363E-24
SrOc	1.848E-38	6.271E-36	4.708E-34	7.999E-33	3.722E-32	3.756E-32	8.441E-33	5.536E-34	1.106E-35	6.576E-38
SrI2c	1.030E-53	3.497E-51	2.626E-49	4.461E-48	2.076E-47	2.095E-47	4.708E-48	3.087E-49	6.168E-51	3.667E-53
SrSc

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aerosol densities (kg/m**3) at i = 1 j = 1 time = 1.25000E+03 s

SrUO4c	1.178E-39	3.997E-37	3.001E-35	5.099E-34	2.373E-33	2.394E-33	5.381E-34	3.528E-35	7.050E-37	4.192E-39
SrMoO4c	3.589E-34	1.218E-31	9.146E-30	1.554E-28	7.231E-28	7.297E-28	1.640E-28	1.075E-29	2.148E-31	1.277E-33
SnC	2.131E-27	7.232E-25	5.430E-23	9.225E-22	4.293E-21	4.332E-21	9.735E-22	6.384E-23	1.276E-24	7.584E-27
SnO2c	2.938E-20	9.971E-18	7.486E-16	1.272E-14	5.919E-14	5.973E-14	1.342E-14	8.802E-16	1.759E-17	1.046E-19
SnI2c	1.079E-49	3.690E-47	2.771E-45	4.708E-44	2.211E-43	2.211E-43	4.968E-44	3.258E-45	6.509E-47	3.870E-49
SnTec	1.579E-45	5.358E-43	4.023E-41	6.836E-40	3.181E-39	3.210E-39	7.213E-40	4.730E-41	9.451E-43	5.620E-45
Tec	5.936E-20	2.015E-17	1.513E-15	2.570E-14	1.196E-13	1.207E-13	2.712E-14	1.778E-15	3.553E-17	2.113E-19
TeO2c	5.285E-23	1.794E-20	1.347E-18	2.289E-17	1.065E-16	1.075E-16	2.415E-17	1.584E-18	3.164E-20	1.881E-22
UO2c
Uc
U4O9c
U3O8c
UO3c
Moc	9.576E-50	3.250E-47	2.440E-45	4.146E-44	1.929E-43	1.947E-43	4.375E-44	2.869E-45	5.732E-47	3.408E-49
MoO2c	7.645E-34	2.595E-31	1.948E-29	3.310E-28	1.540E-27	1.554E-27	3.493E-28	2.290E-29	4.576E-31	2.721E-33
MoO3c	1.497E-35	5.082E-33	3.815E-31	6.483E-30	3.016E-29	3.044E-29	6.841E-30	4.486E-31	8.963E-33	5.329E-35
Agc	1.081E-19	3.670E-17	2.756E-15	4.682E-14	2.179E-13	2.198E-13	4.940E-14	3.240E-15	6.473E-17	3.849E-19
Ag2Tec	7.576E-44	2.571E-41	1.931E-39	3.280E-38	1.526E-37	1.540E-37	3.461E-38	2.270E-39	4.535E-41	2.697E-43
Cdc	2.748E-36	9.326E-34	7.002E-32	1.190E-30	5.536E-30	5.586E-30	1.255E-30	8.233E-32	1.645E-33	9.780E-36
CdOc	2.616E-31	8.880E-29	6.667E-27	1.133E-25	5.271E-25	5.319E-25	1.195E-25	7.839E-27	1.566E-28	9.313E-31
CdTec	6.355E-44	2.157E-41	1.619E-39	2.752E-38	1.280E-37	1.292E-37	2.903E-38	1.904E-39	3.804E-41	2.262E-43
Inc	1.684E-47	5.716E-45	4.292E-43	7.292E-42	3.393E-41	3.424E-41	7.695E-42	5.046E-43	1.008E-44	5.995E-47
In2O3c	1.605E-64	5.447E-62	4.090E-60	6.949E-59	3.234E-58	3.263E-58	7.333E-59	4.809E-60	9.608E-62	5.713E-64
InTec	9.567E-57	3.247E-54	2.438E-52	4.142E-51	1.927E-50	1.945E-50	4.371E-51	2.866E-52	5.727E-54	3.405E-56
Ruc
RuO2c	4.066E-22	1.380E-19	1.036E-17	1.761E-16	8.193E-16	8.267E-16	1.858E-16	1.218E-17	2.434E-19	1.447E-21
Sbc	2.260E-26	7.671E-24	5.760E-22	9.786E-21	4.553E-20	4.595E-20	1.033E-20	6.772E-22	1.353E-23	8.045E-26
Sb2O3c	2.829E-77	9.602E-75	7.209E-73	1.225E-71	5.700E-71	5.752E-71	1.293E-71	8.476E-73	1.694E-74	1.007E-76
Sb2Te3c

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Snc	2.239E-36	1.149E-39
SnOc	1.329E-29	6.821E-33
SnO2c	1.832E-22	9.405E-26
SnI2c	6.782E-52	3.481E-55
SnTec	9.848E-48	5.054E-51
Tec	3.702E-22	1.900E-25
TeO2c	3.297E-25	1.692E-28
UO2c	.	.
Uc	.	.
U4O9c	.	.
U3O8c	.	.
UO3c	.	.
Noc	5.973E-52	3.065E-55
MoO2c	4.768E-36	2.447E-39
1	Test Problem (NEB)	
MoO3c	9.339E-38	4.793E-41
Agc	6.745E-22	3.462E-25
Ag2Tec	4.725E-46	2.425E-49
Cdc	1.714E-38	8.796E-42
CdOc	1.632E-33	8.376E-37
CdTec	3.964E-46	2.034E-49
Inc	1.050E-49	5.391E-53
In2O3c	1.001E-66	5.138E-70
InTec	5.967E-59	3.063E-62
Ruc	.	.
RuO2c	.	.
Sbc	2.536E-24	1.302E-27
Sb2O3c	1.410E-28	7.235E-32
Sb2Te3c	1.765E-79	9.056E-83
Euc	.	.
EuOc	.	.
Eu2O3c	.	.
Cs2U4O12c	.	.
Cs2Tec	4.246E-31	2.179E-34
Cs2TeO3c	6.375E-24	3.272E-27
Cs2Te2O5c	2.299E-38	1.180E-41
Cs2Te4O9c	3.969E-70	2.037E-73
Cs2TeO4c	3.248E-28	1.667E-31
Cs2Te4O12c	9.026E-89	4.632E-92
BaH2c	7.936E-53	4.073E-56
SrH2c	1.450E-56	7.444E-60
TeI4c	1.049E-66	5.386E-70
TeH2O4c	4.138E-35	2.124E-38
UH4O5c	.	.
MoI4c	6.838E-86	3.510E-89
MoI3c	1.192E-74	6.119E-78
MoI2c	6.639E-67	3.407E-70
AgIc	5.590E-28	2.869E-31
CdI2c	5.101E-48	2.618E-51
InIc	5.482E-52	2.814E-55
Ru3Uc	.	.
RuTe2c	.	.
total	2.683E-13	1.377E-16

Description of VICTORIA Output

7.1.9 Aerosol Summary

Following the table of aerosol densities is a table summarizing aerosol behavior. Only the data for the node $i=1$, $j=1$ are included here. The first three columns of data in this table list the masses of each species that deposit as aerosol on ceiling, wall, and floor surfaces. The next column of data provides the total mass on the surface, which includes not only aerosol deposition but also vapor condensation and revaporization of deposits.

The next two columns of data list the resuspension and net deposition rates. The resuspension rate is for mechanical resuspension of previously deposited aerosols. In the current example, both rates are negligible.

The three subsequent columns of data provide information on the size distribution of the aerosols. The first of these columns gives the mass median diameter of the aerosol size distribution. The second column gives the geometric standard deviation. The third column gives the geometric mean diameter. The definitions of these parameters are given in Section 5.8 of this report.

The final column of this table gives the particle concentration for each species. These values are calculated by assuming that the aerosol particles are composed of the pure species at its specified mass concentration. Totals for each column are given at the bottom of the table.

Description of VICTORIA Output

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aerosol summary at i = 1 j = 1 time = 1.25000E+03 s

	deposited mass (kg)		total mass	mass	net	deposition	median	geometric	geometric	particle
	ceiling	wall	on surface	resusp.	rate (kg/s)	rate (kg/s)	diameter	standard deviation	mean diameter	conc. (/m**3)
CsIc	.	1.845E-05	2.588E-04	5.475E-05	.	.	1.147E-07	1.879E+00	3.367E-08	3.279E+14
CsOHC	.	1.859E-05	2.594E-04	4.405E-05	.	.	1.147E-07	1.879E+00	3.367E-08	3.279E+14
Csc	.	1.722E-06	2.141E-05	2.786E-15	.	.	1.147E-07	1.879E+00	3.367E-08	9.750E+03
Cs2Oc	.	7.042E-17	9.316E-16	1.131E-20	.	.	1.147E-07	1.879E+00	3.367E-08	1.278E-03
Cs2UO4c	.	1.500E-23	1.894E-22	2.636E-15	.	.	1.147E-07	1.879E+00	3.367E-08	.
Cs2UO7c	.	3.820E-28	4.794E-27	1.442E-24	.	.	1.147E-07	1.879E+00	3.367E-08	.
Cs2MoO4c	.	1.827E-15	2.423E-14	9.315E-09	.	.	1.147E-07	1.879E+00	3.367E-08	5.928E-02
BaO2H2c	.	2.654E-10	3.196E-09	5.710E-07	.	.	1.147E-07	1.879E+00	3.367E-08	2.996E+04
BaOc	.	9.085E-09	1.04E-07	5.311E-09	.	.	1.147E-07	1.879E+00	3.367E-08	2.786E+02
BaI2c	.	8.387E-14	1.013E-12	8.859E-18	.	.	1.147E-07	1.879E+00	3.367E-08	3.010E-07
Bac	.	1.731E-13	2.110E-12	4.321E-35	.	.	1.147E-07	1.879E+00	3.367E-08	1.305E-24
BaTec	.	6.780E-19	8.361E-18	4.103E-24	.	.	1.147E-07	1.879E+00	3.367E-08	5.797E-21
BaUO4c	.	1.078E-19	1.337E-18	1.398E-10	.	.	1.147E-07	1.879E+00	3.367E-08	.
BaMoO4c	.	1.715E-18	2.194E-17	5.765E-14	.	.	1.147E-07	1.879E+00	3.367E-08	1.704E-13
SrO2H2c	.	1.835E-09	2.208E-08	1.360E-06	.	.	1.147E-07	1.879E+00	3.367E-08	2.095E+02
SrOc	.	1.679E-08	2.024E-07	1.269E-07	.	.	1.147E-07	1.879E+00	3.367E-08	1.955E+01
SrI2c	.	8.875E-15	1.071E-13	1.750E-21	.	.	1.147E-07	1.879E+00	3.367E-08	1.746E-13
SrC	.	1.649E-14	1.995E-13	1.098E-36	.	.	1.147E-07	1.879E+00	3.367E-08	9.736E-29
SrUO4c	.	1.368E-20	1.659E-19	5.014E-11	.	.	1.147E-07	1.879E+00	3.367E-08	.
SrMoO4c	.	1.552E-19	1.962E-18	1.282E-12	.	.	1.147E-07	1.879E+00	3.367E-08	1.112E-14
SnC	.	1.333E-08	1.612E-07	4.147E-20	.	.	1.147E-07	1.879E+00	3.367E-08	3.391E-09
SnOc	.	5.530E-10	6.685E-09	1.417E-13	.	.	1.147E-07	1.879E+00	3.367E-08	2.013E-02
SnO2c	.	6.986E-11	8.435E-10	1.125E-06	.	.	1.147E-07	1.879E+00	3.367E-08	2.776E+05
SnI2c	.	1.504E-16	1.819E-15	1.117E-35	.	.	1.147E-07	1.879E+00	3.367E-08	1.027E-24
SnTec	.	2.931E-16	3.571E-15	3.899E-24	.	.	1.147E-07	1.879E+00	3.367E-08	1.492E-20
Tec	.	8.664E-09	1.067E-07	6.368E-08	.	.	1.147E-07	1.879E+00	3.367E-08	5.609E+05
TeO2c	.	7.394E-15	9.020E-14	1.879E-11	.	.	1.147E-07	1.879E+00	3.367E-08	4.994E+02
UO2c	.	2.668E-12	3.305E-11	6.699E-14	.	.	1.147E-07	1.879E+00	3.367E-08	.
Uc	.	3.684E-22	4.544E-21	3.246E-64	.	.	1.147E-07	1.879E+00	3.367E-08	.
U4O9c	.	2.974E-48	3.729E-47	5.788E-54	.	.	1.147E-07	1.879E+00	3.367E-08	.
U3O8c	.	3.862E-40	4.812E-39	1.740E-42	.	.	1.147E-07	1.879E+00	3.367E-08	.
UO3c	.	8.220E-16	1.017E-14	3.711E-16	.	.	1.147E-07	1.879E+00	3.367E-08	.
Moc	.	3.975E-11	5.036E-10	4.472E-34	.	.	1.147E-07	1.879E+00	3.367E-08	9.046E-25
MoO2c	.	9.081E-12	1.152E-10	1.183E-18	.	.	1.147E-07	1.879E+00	3.367E-08	7.221E-09
MoO3c	.	7.000E-13	8.839E-12	1.334E-20	.	.	1.147E-07	1.879E+00	3.367E-08	1.414E-10
Agc	.	2.694E-06	1.625E-05	6.786E-05	.	.	1.147E-07	1.879E+00	3.367E-08	1.022E+06
Ag2Tec	.	1.310E-06	3.421E-21	1.271E-11	.	.	1.147E-07	1.879E+00	3.367E-08	7.167E-19
CdOc	.	8.890E-09	1.062E-07	4.161E-22	.	.	1.147E-07	1.879E+00	3.367E-08	2.597E-11
CdTec	.	1.934E-08	2.290E-07	2.281E-17	.	.	1.147E-07	1.879E+00	3.367E-08	2.473E-06
CdOc	.	1.226E-18	1.464E-17	2.057E-22	.	.	1.147E-07	1.879E+00	3.367E-08	6.006E-19
Inc	.	5.543E-19	6.709E-18	1.125E-42	.	.	1.147E-07	1.879E+00	3.367E-08	1.592E-22
In2O3c	.	6.728E-32	7.928E-31	2.724E-60	.	.	1.147E-07	1.879E+00	3.367E-08	1.518E-39
InTec	.	2.846E-29	3.449E-28	1.366E-44	.	.	1.147E-07	1.879E+00	3.367E-08	9.043E-32
Ruc	.	2.623E-13	3.277E-12	1.128E-11	.	.	1.147E-07	1.879E+00	3.367E-08	.

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Test Problem (NEB)

Description of VICTORIA Output

aerosol summary at i = 1 j = 1 time = 1.25000E+03 s

	deposited mass (kg)		total mass on surface (kg)	mass resusp. rate (kg/s)	net deposition rate (kg/s)	mass median diameter	geometric standard deviation	geometric mean diameter	particle conc. (/m**3)
	ceiling	wall	floor						
RuO2c	.	1.359E-19	1.682E-18	1.390E-15	.	1.147E-07	1.879E+00	3.367E-08	.
Sbc	.	3.891E-10	4.803E-09	2.034E-10	.	1.147E-07	1.879E+00	3.367E-08	3.842E+03
Sb2O3c	.	2.392E-18	2.858E-17	2.150E-08	.	1.147E-07	1.879E+00	3.367E-08	2.136E-01
Sb2Te3c	.	4.886E-48	5.983E-47	1.377E-36	.	1.147E-07	1.879E+00	3.367E-08	2.673E-52
Euc	.	1.562E-14	1.889E-13	3.743E-44	.	1.147E-07	1.879E+00	3.367E-08	.
EuOc	.	2.128E-09	2.568E-08	7.220E-18	.	1.147E-07	1.879E+00	3.367E-08	.
Eu2O3c	.	2.390E-10	2.861E-09	1.705E-07	.	1.147E-07	1.879E+00	3.367E-08	.
Cs2U4O12c	.	2.534E-61	3.256E-60	1.460E-48	.	1.147E-07	1.879E+00	3.367E-08	.
Cs2Tec	.	1.248E-14	9.354E-13	2.114E-13	.	1.147E-07	1.879E+00	3.367E-08	6.433E-04
Cs2TeO3c	.	1.016E-19	2.479E-18	6.054E-07	.	1.147E-07	1.879E+00	3.367E-08	9.657E+03
Cs2Te2O5c	.	4.434E-34	9.618E-33	1.547E-14	.	1.147E-07	1.879E+00	3.367E-08	3.483E-11
Cs2Te4O9c	.	8.361E-62	9.993E-61	1.339E-32	.	1.147E-07	1.879E+00	3.367E-08	6.012E-43
Cs2TeO4c	.	1.734E-22	2.136E-21	1.776E-11	.	1.147E-07	1.879E+00	3.367E-08	4.920E-01
Cs2Te4O12c	.	1.189E-74	1.421E-73	5.810E-52	.	1.147E-07	1.879E+00	3.367E-08	1.367E-61
BaH2c	.	7.725E-18	9.352E-17	6.913E-36	.	1.147E-07	1.879E+00	3.367E-08	1.202E-25
SrH2c	.	4.734E-18	5.726E-17	4.303E-37	.	1.147E-07	1.879E+00	3.367E-08	2.197E-29
TeI4c	.	7.089E-38	8.643E-37	1.426E-52	.	1.147E-07	1.879E+00	3.367E-08	1.590E-39
TeH2O4c	.	1.814E-22	2.176E-21	1.357E-21	.	1.147E-07	1.879E+00	3.367E-08	6.268E-08
UH4O5c	.	1.193E-18	1.450E-17	2.054E-21	.	1.147E-07	1.879E+00	3.367E-08	.
MoI4c	.	2.480E-35	3.106E-34	4.046E-68	.	1.147E-07	1.879E+00	3.367E-08	1.036E-58
MoI3c	.	2.272E-28	2.852E-27	7.482E-57	.	1.147E-07	1.879E+00	3.367E-08	1.806E-47
MoI2c	.	4.738E-22	5.960E-21	4.419E-49	.	1.147E-07	1.879E+00	3.367E-08	1.005E-39
AgIc	.	1.996E-10	2.459E-09	5.303E-11	.	1.147E-07	1.879E+00	3.367E-08	8.473E-01
CdI2c	.	9.382E-16	1.118E-14	1.101E-31	.	1.147E-07	1.879E+00	3.367E-08	7.729E-21
InIc	.	2.265E-21	2.740E-20	5.538E-45	.	1.147E-07	1.879E+00	3.367E-08	8.308E-25
Ru3Uc	.	2.701E-55	3.440E-54	5.858E-85	.	1.147E-07	1.879E+00	3.367E-08	.
RuTe2c	.	6.843E-30	8.487E-29	2.572E-17	.	1.147E-07	1.879E+00	3.367E-08	.
total	.	4.016E-05	5.569E-04	1.707E-04	.	1.147E-07	1.879E+00	3.367E-08	6.558E+14

Description of VICTORIA Output

7.1.10 Deposition Velocities

Aerosol deposition velocities characterize the importance of each of the deposition mechanisms that are modeled by VICTORIA. Each of these deposition velocities is discussed in Section 5.6 of this report. Deposition velocities are given for each collocation point so that variations with particle size can be understood. For brevity, data are included only for the node $i=1$, $j=1$.

In this example the flow regime is turbulent, so the laminar deposition velocity is 0. No flow irregularities were prescribed in the input for this node, so the bend deposition velocity is zero. Thermophoretic deposition velocities are negligible because there is no temperature gradient between the gas and the structural surfaces. Turbulent deposition velocity is greater than gravitational settling velocity for smaller particles, but the role of the two mechanisms is switched for the larger particles. Overall, gravitational settling is slightly more important than turbulent deposition for this example, as seen from the last column of data. This column gives the weighted average deposition velocity, which is calculated by weighting the deposition velocity for each aerosol size by the fraction of the aerosols in that size class.


```

deposition velocities (m/s) at i = 1 j = 1 time = 1.25000E+03 s
collocation points
mass (kg) 1.0E-22 1.0E-21 1.0E-20 1.0E-19 1.0E-18 1.0E-17 1.0E-16 1.0E-15 1.0E-14 1.0E-13
radius (m) 1.8E-09 3.9E-09 8.4E-09 1.8E-08 3.9E-08 8.4E-08 1.8E-07 3.9E-07 8.4E-07 1.8E-06
laminar
turb 3.696E-04 1.136E-04 3.867E-05 1.384E-05 5.132E-06 2.001E-06 8.503E-07 4.082E-07 2.264E-07 1.779E-07
thermo
gravity 1.318E-07 2.857E-07 6.235E-07 1.381E-06 3.159E-06 7.727E-06 2.142E-05 7.074E-05 2.729E-04 1.152E-03
bend(/s) . . . . . . . . . .
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deposition velocities (m/s) at i = 1 j = 1 time = 1.25000E+03 s
mass (kg) 1.0E-12 1.0E-11 weighted
radius (m) 3.9E-06 8.4E-06 average
laminar
turb 3.551E-07 1.469E-06 4.370E-06
thermo
gravity 5.104E-03 2.316E-02 6.960E-06
bend(/s) . . .

```

Description of VICTORIA Output

7.1.11 Total Element Masses

Total element masses are given in tabular format for all of the nodes, i.e., for the entire domain. These data are broken down by subregion in the same way as the element masses for an individual node.

This data table provides a complete mass balance for each element. The column of data labeled "total" gives the total mass of each element contained in the domain at the current time step. The subsequent four columns provide data on the mass of each element that enters the domain as a source or leaves the domain as an effluent; these data are characterized as either gases or aerosols. Following these columns is one labeled "initial," which gives the mass of each element contained within the domain at the beginning of the calculation. The following column, labeled "balance," give the mass balance error, which is calculated from the equation:

$$\text{balance} = \text{total} + \text{lost gas} + \text{lost aero} - \text{initial} - \text{gas sce} - \text{aero sce} \quad (7.1)$$

When this quantity is positive, mass was created due to numerical errors; when this quantity is negative, mass was lost due to numerical errors. The next column of data contains a relative measure of error. This error is expressed in the following way:

$$\frac{\text{balance}}{\text{initial} + \text{gas sce} + \text{aero sce}} = \frac{\text{total} + \text{lost gas} + \text{lost aero}}{\text{initial} + \text{gas sce} + \text{aero sce}} - 1 \quad (7.2)$$

which is the final mass divided by the initial mass minus 1. In this example, the relative errors on all of the mass balances are less than 1%, with the single exception of tin. Generally, the mass balance errors should be small for all of the elements.

The final column of data in this table gives fractional releases of fission products from fuel. Fission products are considered to be released from the fuel once they reach the bulk gas in the coolant channel.

Description of VICTORIA Output

element masses (kg) in all cells at time = 1.25000E+03 s

element	grains	pores	gap	clad	film	control	bulk gas	aerosol	structure	total
Ba	5.497E-04	3.032E-03	7.639E-05	4.453E-14	3.071E-13	1.355E-08	3.156E-23	2.663E-10	2.274E-05	3.681E-03
Cs	9.948E-04	4.249E-04	2.406E-04	1.726E-09	9.111E-09	6.710E-07	4.314E-09	1.409E-03	7.043E-03	1.011E-02
H	.	2.200E-06	2.832E-06	6.159E-06	7.457E-05	1.387E-05	4.485E-01	6.708E-06	4.836E-03	4.534E-01
I	7.326E-05	3.233E-05	4.826E-05	3.144E-12	9.710E-11	7.009E-07	6.011E-12	4.942E-04	3.693E-03	4.342E-03
Mo	1.144E-03	7.996E-03	1.398E-08	1.936E-18	2.189E-17	3.271E-11	9.671E-26	1.173E-12	2.125E-08	9.139E-03
O	6.168E-01	6.377E-04	5.628E-05	1.657E-01	5.959E-04	1.110E-04	3.588E+00	1.073E-04	3.890E-02	4.411E+00
Ru	8.466E-04	5.919E-03	1.575E-10	.	9.102E-29	1.752E-13	2.662E-43	1.374E-18	1.659E-10	6.766E-03
Sn	1.807E-05	7.452E-05	5.671E-06	9.008E-03	4.372E-12	2.268E-08	5.518E-32	3.361E-11	2.305E-05	9.129E-03
Sr	3.557E-04	6.549E-04	3.347E-04	2.091E-16	1.489E-15	3.283E-08	2.534E-29	2.005E-12	4.866E-05	1.394E-03
Te	1.538E-04	6.579E-04	3.413E-07	1.365E-11	6.993E-12	5.666E-09	1.511E-18	5.858E-09	6.147E-06	8.182E-04
U	4.560E+00	1.249E-10	2.869E-05	4.812E-26	4.343E-25	1.496E-12	5.817E-47	2.953E-20	1.641E-09	4.560E+00
Zr	1.054E-02	.	.	5.540E-01	5.645E-01
B
Fe
Cr
Mn
Ni
Ag	.	2.557E-08	1.813E-07	7.182E-13	8.106E-12	4.304E-02	1.108E-21	4.305E-07	1.109E-03	4.415E-02
In	.	2.112E-17	4.110E-17	4.059E-21	2.211E-20	2.825E-24	1.707E-19	1.322E-37	2.886E-21	6.242E-17
Cd	.	3.784E-13	9.255E-13	2.102E-19	1.221E-18	1.106E-16	9.520E-21	1.277E-12	1.244E-07	1.244E-07
Sb	6.954E-06	2.830E-05	3.153E-07	1.002E-14	5.748E-14	4.374E-10	1.424E-25	1.455E-12	4.293E-07	3.600E-05
Bu	5.496E-05	1.344E-04	3.626E-05	7.667E-17	5.019E-16	4.492E-09	1.604E-49	2.091E-15	7.113E-06	2.328E-04
Kr	1.382E-04	1.037E-06	2.024E-06	1.700E-10	8.315E-10	1.396E-13	8.439E-09	.	1.426E-10	1.413E-04
Xe	1.899E-03	1.427E-05	2.786E-05	2.590E-09	1.359E-08	1.918E-12	1.159E-07	.	1.959E-09	1.941E-03
He	.	1.538E-08	3.014E-08	1.767E-12	5.681E-12	2.315E-15	1.399E-10	.	2.357E-12	4.566E-08
Ar

element masses (kg) in all cells at time = 1.25000E+03 s

element	lost gas	gas sce	lost aero	aero sce	initial	balance	bal/init+sce	rls/init
Ba	4.148E-07	.	6.986E-04	.	4.393E-03	-1.333E-05	0.003035	0.164296
Cs	5.386E-02	.	8.172E-01	8.738E-01	7.951E-03	-6.327E-04	0.000718	0.997399
H	1.102E+02	1.073E+02	3.814E-03	4.169E-03	3.400E+00	2.076E-04	0.000002	1.000001
I	1.127E-02	.	2.890E-01	3.053E-01	5.855E-04	-1.279E-03	0.004183	0.995312
Mo	3.689E-11	.	9.558E-07	.	9.140E-03	-2.191E-08	0.000002	0.000107
O	7.487E+02	7.253E+02	6.166E-02	6.671E-02	2.774E+01	1.537E-03	0.000002	0.998961
Ru	3.087E-13	.	6.496E-09	.	6.766E-03	-1.356E-10	0.000000	0.000001
Sn	4.063E-07	.	9.474E-04	.	1.298E-02	-2.903E-03	0.223659	0.074792
Sr	1.896E-07	.	1.423E-03	.	2.842E-03	-2.485E-05	0.008742	0.517947
Te	1.618E-06	.	4.044E-04	.	1.229E-03	-4.881E-06	0.003971	0.335319
U	1.974E-12	.	5.609E-08	.	4.560E+00	-1.264E-09	0.000000	0.000000
Zr	5.645E-01	5.551E-16	0.000000	.
B
Fe
Cr
Mn
Ni
Ag	6.486E-06	.	3.235E-02	.	.	7.651E-02	.	.
In	1.321E-02	.	7.322E-14	.	.	1.321E-02	.	.
Cd	1.332E-03	.	4.404E-03	.	.	5.736E-03	.	.
Sb	9.384E-09	.	1.927E-05	.	5.557E-05	-2.935E-07	0.005281	0.354615
Bu	2.490E-08	.	2.026E-04	.	4.392E-04	-3.840E-06	0.008742	0.477515
Kr	9.633E-04	.	.	.	1.105E-03	1.079E-09	0.000001	0.872102
Xe	1.324E-02	.	.	.	1.518E-02	1.377E-08	0.000001	0.872097
He	2.531E-04	.	.	.	2.532E-04	2.846E-10	0.000001	0.999821
Ar

Description of VICTORIA Output

7.1.12 CPU Timings

The final information in the output file contains CPU timing information. For this example, 2600 time steps were taken. The total CPU time required for the calculation was 5827 s. Of this time, about 180 s were spent on calculating fission product release from fuel, 2367 s on chemistry calculations, 816 on gas transport, 1835 s on aerosol agglomeration and deposition, 120 s on decay heating, 144 s on aerosol transport, and 256 s to determine diffusion of species to and from boundary layers. About 109 of the 5827 s are consumed in miscellaneous calculations that do not show up in any of the categories.

```
0   current CPU timings are:  istep   total   fuel    chem   gas tran  aero   decay aer tran  bndy-dif
                             2600    5827.1   180.1   2367.4   816.2  1835.4   119.7   143.8   255.8
```

7.1.13 Messages

Many of the messages that can appear in the output file also appear in the progress file, which is discussed in Section 7.2. Because it is usually easier to scan through the progress file, the messages that are common to both files are described in Section 7.2 but not here; only the messages that only appear in the output file are described in this subsection. All of these error messages are triggered by errors in the input file. These input error messages are categorized as syntax errors, dimension errors, and range errors. The messages that fall into each of these categories are discussed below. Most of the errors described in this subsection terminate code execution.

Syntax Errors

```
species in aerosol source to bulk gas      CsZrc does not exist  ** ERROR
```

This message indicates that the user has tried to input an aerosol species that does not exist in the VICTORIA database.

```
Input error - card read in is not a keyword card
Read from next keyword data set
```

This message indicates that a keyword, i.e., descriptor, was expected but what was read was not a keyword. This could indicate that the keyword was misspelled or out of place.

```
-- CARD IMAGE NOT READ BY VICTORIA --
```

This message indicates that the sequence or format of the input deck is incorrect and that the input reader cannot interpret the current line of information. Generally, this message appears until the next keyword is read.

```
***** Input deck is incorrect *****      unknown keyword being input
```

This message indicates that a keyword is misspelled.

```
-- UNKNOWN FISSION PRODUCT ELEMENT --
```

Description of VICTORIA Output

This message indicates that a fission product element prescribed in the fuel inventory is not in the VICTORIA database. Commonly, this is due to a misspelling or other syntax error.

```
KEYWORD      **TDEPSRCE      data set is missing
```

This message indicates that the data that should accompany a keyword is missing.

```
INSS input processing completed - - - correct errors noted above, then resubmit
```

This message indicates that errors were encountered while processing the static portion of the input file, i.e., the portion prior to the PAUSE command. The errors should be corrected before resubmitting the run.

```
Input error detected while processing data set  TDEPSTRU
Probable lack of data in this input block
Read until next keyword data set
```

This message indicates that the input file reader did not find information in the expected format or order. A common reason for this message is that one or more parameters were omitted from the input file.

```
Unexpected end of file detected while processing keyword data set
```

This message indicates that the end of the input file was reached before all of the expected input was read.

```
Unknown keyword detected after processing data set TDEPSTRU
Read from next keyword data set
```

This message indicates that a keyword was not recognized. When this occurs, the input reader searches for the next keyword and continues processing the input file.

```
No fuel rods (irodr = 0). Fuel data ignored.
```

This message indicates that fuel data were provided even though the fission product release flag was set to zero, i.e., no fission product release is to be calculated. When this happens, the fuel data are ignored.

```
species in vapor source to bulk gas    CsZrc does not exist  ** ERROR
```

This message indicates that a vapor species was specified as a vapor source that does not exist in the thermochemical database.

```
INTS input processing completed - - - correct errors noted above, then resubmit
```

This message indicates that errors were encountered while processing the transient block of input data. These errors must be corrected before the calculation can be run.

Dimension Errors

```
Input values are incompatible with those in this version of VICTORIA - -
jmax,imax,nfuel,nclad may not exceed    30    4    2    1
```

Description of VICTORIA Output

This message indicates that one or more of indicated dimensions in VICTORIA is smaller than the value requested by the user. The default maximum dimensions allowed are 30 axial levels, 4 radial rings, 2 fuel subnodes, and 1 fuel cladding subnode. These dimensions can be modified and the code recompiled if larger values are needed.

```
**** Input error ****  
nse = 25 greater than parameter lsrce = 20
```

This message indicates that too many aerosol sources were included in the input file. The default maximum is 20. The maximum can be increased and the code recompiled.

```
**** Input error ****  
nstval = 400 greater than parameter lstval = 300
```

The default maximum number of time values for aerosol sources is 300. This message indicates that the user exceeded this maximum. The maximum can be increased and the code recompiled.

```
**** Input error ****  
itvals = 500 greater than parameter itime = 400
```

This message indicates that the maximum number of time values for thermal-hydraulic data has been exceeded. The default maximum, which is 400, can be increased and the code recompiled.

```
**** Input error ****  
nfptim = 400 greater than parameter lfptim = 300
```

This message indicates that the maximum number of time values for vapor source data has been exceeded. The default maximum, which is 300, can be increased and the code recompiled.

```
**** Input error ****  
nfpmas = 25 greater than parameter lfpmas = 20
```

This message indicates that the maximum number of vapor sources has been exceeded. The default maximum, which is 20, can be increased and the code recompiled.

Range Errors

```
ERROR clad oxidation fraction is outside limits
```

This message indicates that the user-specified clad oxidation fraction is outside the acceptable range of 0 to 1.

```
gap or clad thickness not zero when there is no clad (nclad=0), code will reset to 0.0
```

This message indicates that cladding data in the input file are inconsistent. No cladding nodes were specified, i.e., the fuel is specified to be unclad, yet the thickness of the cladding was not set to zero. In this situation, the code automatically resets the cladding thickness to zero.

```
Bulk gas thermal hydraulic input requires
```

Description of VICTORIA Output

number of time values (itvals) to be input here
when there is no fuel data.

A common error is to omit the number of time values at the top of the TDEPSTRU section of input data when the TDEPFUEL is not included in the file. The input file reader only expects this additional data only when the TDEPFUEL section is not included in the input file, as discussed in Subsection 6.5.3.

Input error detected while processing data...Time Step is zero

This message indicates that the user accidentally specified a zero time-step size in the input file.

Temperatures too low at j,i= 1 1 time= 1000.00
temps= 350.000 350.000 350.000

The default minimum structure temperature that VICTORIA allows is 400 K. The above message indicates that structure temperatures below this value, for the ceiling, wall, or floor, were prescribed by the user. In some cases, it may be appropriate to reduce this minimum temperature and recompile the code to avoid this error.

Low fuel temperature at j,i= 1 1 time= 1000.00
temps= 850.000 850.000 850.000
should be changed to minimum fuel temp 900.000 K

The default minimum fuel temperature, for fuel centerline, fuel surface, or fuel cladding, that VICTORIA allows is 900 K because lower temperatures can sometimes cause fuel thermochemistry calculations to be nonconvergent. Generally, even if the actual fuel temperatures are lower than this value, they should be reset to 900 K; doing this will not affect predictions because fission product release is negligible at 900 K.

Pressure too low at j,i= 1 1 time= 1000.00
press= 4000.000

The default minimum pressure that VICTORIA allows is 5000 Pa. Specifying a pressure to be less than this minimum will result in the above message. Under unusual conditions where pressures are less than this minimum, it can be lowered and the code recompiled.

volume(1, 1) is calculated to be -1.000000e-01

This message indicates that the input parameters specified by the user result in a non-positive volume being calculated for bulk gas subregion of a node. When this happens, the user should reexamine the input parameters and make necessary corrections.

7.2 Progress File

The progress file contains information on the progress of a calculation. It may also contain warning messages, as it does in this example. Finally, it may contain messages indicating that the numerical procedures are encountering some difficulties. It is good practice for the VICTORIA user to examine this file as the run proceeds and after the run is complete.

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7.2.1 Example

The output for the first 60 time steps of the progress file for the example problem are displayed on the following page. There are several warning messages. The first two warnings indicate that the time step size exceeds the Courant limit, as discussed further in Part IV of this report. In simple terms, the Courant limit is the time step for which gases flow the length of one of nodes during the time step. In this example, the Courant limit is violated for flows in the axial and radial dimensions. To satisfy the Courant limit, the time step should be reduced to about 0.04 s or less. The recommended procedure is to set the time step to no more than half the Courant limit.

A number of messages in the progress file indicate that the numerical procedure is having some difficulty with convergence. These warnings are mild, however, and are not cause for alarm. Some of the messages listed in the following subsection may indicate significant mass balance errors, and thus may require some adjustments in the input to obtain an acceptable solution.

One additional message indicates that one of the control rods fails at 50 s. This message is purely informational. A complete list of the messages that can appear in the progress file is given in the following subsection.

```
WARNING: time step 1.0000E+00 exceeds Courant limit axially at j= 6. Axial limit is 4.1324E-02 seconds
WARNING: time step 1.0000E+00 exceeds Courant limit radially at j= 1, i= 1. Radial limit is 6.6126E-01
seconds
```

```
CHEMISTRY problem: element Te      in cell 7 in pores region ; attempt number 1
CHEMISTRY problem: element Te      in cell 8 in pores region ; attempt number 1
```

Time Step CPU Information									
step number	time	time step	fuel	chem	gas transp	* aerosol * phys transp	decay	boundy layer	
1	1.000	1.000	0.08	0.53	0.13	0.11	0.03	0.04	0.04
2	2.000	1.000	0.07	0.61	0.32	0.74	0.04	0.05	0.25
3	3.000	1.000	0.07	0.40	0.30	0.74	0.05	0.05	0.22
4	4.000	1.000	0.05	0.55	0.26	0.79	0.04	0.05	0.20
5	5.000	1.000	0.08	0.47	0.32	0.95	0.04	0.05	0.29
6	6.000	1.000	0.06	0.45	0.26	0.67	0.04	0.05	0.19
7	7.000	1.000	0.06	0.39	0.25	0.65	0.03	0.04	0.23
CHEMISTRY problem: element Ba in cell 1 in gap region ; attempt number 1									
CHEMISTRY problem: element Ba in cell 2 in gap region ; attempt number 1									
CHEMISTRY problem: element Ba in cell 7 in gap region ; attempt number 1									
CHEMISTRY problem: element Ba in cell 8 in gap region ; attempt number 1									
8	8.000	1.000	0.05	0.54	0.25	0.65	0.03	0.04	0.18
9	9.000	1.000	0.05	0.45	0.23	0.65	0.03	0.04	0.18
10	10.000	1.000	0.05	0.41	0.23	0.66	0.03	0.04	0.18
11	11.000	1.000	0.05	0.40	0.23	0.67	0.03	0.04	0.16
12	12.000	1.000	0.05	0.39	0.22	0.67	0.03	0.04	0.18
13	13.000	1.000	0.05	0.40	0.21	0.67	0.04	0.05	0.17
14	14.000	1.000	0.05	0.39	0.19	0.67	0.03	0.04	0.18
15	15.000	1.000	0.05	0.37	0.22	0.67	0.03	0.04	0.17
16	16.000	1.000	0.05	0.40	0.19	0.67	0.04	0.05	0.16
17	17.000	1.000	0.05	0.40	0.18	0.66	0.03	0.05	0.16
18	18.000	1.000	0.05	0.37	0.19	0.67	0.03	0.04	0.15
19	19.000	1.000	0.05	0.39	0.18	0.68	0.04	0.05	0.15
20	20.000	1.000	0.05	0.40	0.16	0.67	0.03	0.05	0.15
21	21.000	1.000	0.05	0.37	0.19	0.69	0.03	0.04	0.15
22	22.000	1.000	0.05	0.40	0.17	0.68	0.03	0.04	0.14
23	23.000	1.000	0.05	0.41	0.15	0.67	0.03	0.05	0.13
24	24.000	1.000	0.05	0.39	0.15	0.66	0.03	0.04	0.16
25	25.000	1.000	0.05	0.39	0.16	0.68	0.03	0.05	0.14

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26	26.000	1.000	0.05	0.39	0.17	0.68	0.03	0.05	0.15
27	27.000	1.000	0.05	0.40	0.15	0.68	0.03	0.05	0.12
28	28.000	1.000	0.05	0.40	0.17	0.68	0.03	0.05	0.13
29	29.000	1.000	0.05	0.37	0.17	0.69	0.03	0.04	0.14
30	30.000	1.000	0.05	0.39	0.17	0.67	0.03	0.04	0.14
31	31.000	1.000	0.05	0.40	0.15	0.67	0.03	0.04	0.12
32	32.000	1.000	0.05	0.40	0.17	0.67	0.03	0.04	0.13
33	33.000	1.000	0.05	0.36	0.17	0.68	0.03	0.04	0.14
34	34.000	1.000	0.05	0.39	0.17	0.69	0.04	0.04	0.13
35	35.000	1.000	0.05	0.39	0.15	0.68	0.03	0.05	0.13
36	36.000	1.000	0.05	0.38	0.16	0.66	0.03	0.04	0.14
37	37.000	1.000	0.05	0.37	0.17	0.67	0.03	0.05	0.14
38	38.000	1.000	0.05	0.39	0.15	0.67	0.03	0.05	0.12
39	39.000	1.000	0.05	0.39	0.17	0.66	0.03	0.05	0.14
40	40.000	1.000	0.05	0.37	0.18	0.66	0.03	0.04	0.14
41	41.000	1.000	0.05	0.38	0.17	0.69	0.03	0.05	0.13
42	42.000	1.000	0.05	0.39	0.15	0.68	0.03	0.05	0.12
43	43.000	1.000	0.05	0.39	0.16	0.67	0.03	0.04	0.14
44	44.000	1.000	0.05	0.37	0.17	0.68	0.03	0.04	0.14
45	45.000	1.000	0.05	0.36	0.17	0.67	0.03	0.04	0.13
46	46.000	1.000	0.05	0.39	0.16	0.66	0.03	0.05	0.12
47	47.000	1.000	0.05	0.40	0.15	0.65	0.03	0.04	0.13
48	48.000	1.000	0.05	0.39	0.16	0.66	0.03	0.04	0.14
49	49.000	1.000	0.05	0.36	0.17	0.66	0.03	0.04	0.13
Control rod fails in ring 1, axial level 1 at time = 50.0000 seconds.									
CHEMISTRY	problem:	element	In	in cell	1	in control region ; attempt number	1		
50	50.000	1.000	0.05	0.43	0.17	0.66	0.03	0.04	0.12
CHEMISTRY	problem:	element	I	in cell	1	in gas region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	2	in gas region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	3	in gas region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	4	in gas region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	5	in gas region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	6	in gas region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	7	in gas region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	8	in gas region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	9	in gas region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	10	in gas region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	11	in gas region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	12	in gas region ; attempt number	1		
51	51.000	1.000	0.05	0.95	0.18	0.66	0.04	0.05	0.12
CHEMISTRY	problem:	element	I	in cell	1	in structure region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	2	in structure region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	3	in structure region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	4	in structure region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	5	in structure region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	6	in structure region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	7	in structure region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	8	in structure region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	9	in structure region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	10	in structure region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	11	in structure region ; attempt number	1		
CHEMISTRY	problem:	element	I	in cell	12	in structure region ; attempt number	1		
CHEMISTRY	problem:	element	O	in cell	1	in control region ; attempt number	1		
CHEMISTRY	problem:	element	O	in cell	1	in control region ; attempt number	2		
CHEMISTRY	problem:	element	Cs	in cell	1	in control region ; attempt number	3		
CHEMISTRY	problem:	element	I	in cell	2	in control region ; attempt number	1		
CHEMISTRY	problem:	element	O	in cell	7	in control region ; attempt number	1		
CHEMISTRY	problem:	element	O	in cell	8	in control region ; attempt number	1		
52	52.000	1.000	0.05	1.36	0.24	0.67	0.04	0.05	0.17
53	53.000	1.000	0.05	0.56	0.24	0.64	0.04	0.04	0.18
54	54.000	1.000	0.05	0.55	0.23	0.65	0.03	0.04	0.16
55	55.000	1.000	0.06	0.53	0.23	0.66	0.03	0.04	0.14
56	56.000	1.000	0.05	0.51	0.20	0.65	0.03	0.04	0.13
57	57.000	1.000	0.05	0.50	0.19	0.67	0.04	0.04	0.12
58	58.000	1.000	0.05	0.51	0.18	0.66	0.04	0.04	0.11
59	59.000	1.000	0.05	0.51	0.17	0.67	0.03	0.04	0.10
60	60.000	1.000	0.05	0.52	0.15	0.66	0.04	0.05	0.09

7.2.2 Messages

A number of messages can appear in the progress file. These messages can be categorized as termination messages, warnings, problems, and information. The first category,

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termination messages, indicates a problem has occurred that caused a numerical algorithm to fail and that no recovery was possible. The second category, warnings, may require user attention to correct a problem but does not result in termination of the run. Problem messages are milder than warnings; they usually indicate some mild difficulties with numerical convergence from which the algorithm was able to recover. They usually do not indicate that any significant errors have occurred. The final category, information, indicates events that occur during the calculation. These messages are intended to help the user better understand the results. Messages that fall under each of the categories are described below.

Termination Messages

```
*** AROFLO fails: IFAIL is 2 i = 1 j = 1 ***
```

There is no simple fix for the problem that generates this message. If it appears, please report it to the VICTORIA developers.

```
*** AROMOM fails: IFAIL is 2 i = 1 j = 1 ***
```

This message usually indicates that the range of aerosol sizes defined in the input is inappropriate for the problem. Most commonly, the minimum aerosol size needs to be reduced.

```
*** AROSLV fails - not enough storage allocated
    number of eqns = 20    parameter idm in AROSLV must be increased to 50
*** AROSLV fails: IDID is 2 i = 1 j = 1 ***
*** AROZER fails: interval does not contain a zero ***
*** AROZER fails: zero not found after 20 steps i = 1 j = 1 ***
*** AROZER fails: IDID = 20 i = 1 j = 1 ***
```

There is no simple fix for the problems that generate these messages. If one of them appears, please report it to the VICTORIA developers.

```
*** INAERO warning: end-of-file read - error in the data ****
```

This message indicates an error in the AERODATA portion of the input file, as described in Subsection 6.3.7. Usually, one or more parameters are missing from the input.

```
*** BDIO: Error in boundary file name    test.bdy
```

This message indicates there is a problem with the subdomain coupling file that is being read, as described in Subsection 6.5.6.

```
*** SAROCO fails: YLOWER is ge YUPPER ***
*** SAROIN fails: NONZERO is 1 ***
```

There is no simple fix for the problems that generate these messages. If one of them appears, please report it to the VICTORIA developers.

```
Warning *    error reading boundary file
```

This message indicates there is a problem with the subdomain coupling file that is being read, as described in Subsection 6.5.6.

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WARNING: relative error in pressure 51.0% exceeds 20% at j= 1, i= 1. Time of occurrence is 1000.0000 seconds

This message indicates that the thermal-hydraulic data are inconsistent; these data are described in Subsection 6.5.3. Using the data would result in a pressure in one of the nodes that is at least 50% too large or too small, compared with the input value. When this message appears, the user needs to reexamine the thermal-hydraulic input data and correct the errors.

Warnings

```
CHEMISTRY retry: element      Cs in cell 1 in bulk gas region ; liq fr = 0.10000e+00
CHEMISTRY failed: element     Cs in cell 1 in bulk gas region ; error = 0.10000e+00
CHEMISTRY failed: element     Cs in cell 1 in bulk gas region ; mass error = 0.10000e+00
```

These errors indicate that convergence of the numerical algorithm used to determine thermochemical equilibrium failed. These failures almost always result in mass balance errors, which are discussed in Subsection 7.1.11, although these mass balance errors are not always significant. If any of these messages appear in the progress file, the user should carefully examine the mass balance error data in the output file. If mass balance errors are unacceptably large, the user should reduce the time-step size and repeat the run. This may fix the problem, but is not guaranteed to do so.

```
Frozen chemistry not converged in cell 1 in bulk gas region; csum = 0.10000e+00
```

This message indicates that the frozen chemistry algorithm failed to converge. This will not usually result in a mass balance error, but may result in an error in the relative masses of a species that is in the condensed and vapor phases. The solution to this problem may be to reduce the time-step size, although there is no guarantee that this will help.

```
**** Function POLATE warning **** X value ( 0.0) less than minimum ( 0.1)
**** Function POLATE warning **** X value ( 2.0) more than maximum ( 1.0)
```

This message indicates that the program was trying to interpolate data outside the range specified in the input file. This usually indicates an error in the transient data, such as temperatures, pressures, flow rates, or mass source rates, in the input data.

```
*** SAROCO warning: IERROR is 1 ***
```

There is no simple fix for the problems that generate these messages. If one of them appears, please report it to the VICTORIA developers.

```
SPOFS failed: message number 1 reverting to cyclic Newton method in CHMGAS:
element      Cs in cell 1 in bulk gas region
SPOFS warning: message number 1 in CHMGAS:
element      Cs in cell 1 in bulk gas region
```

These messages indicate convergence problems with the numerical algorithm used to determine thermochemical equilibrium. These messages usually do not indicate serious problems.

```
WARNING: time step 1.0000E+00 exceeds Courant limit axially at j= 6. Axial limit is 4.1324E-02 seconds
```

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```
WARNING: time step 1.0000E+00 exceeds Courant limit radially at j= 1, i= 1. Radial limit is 6.6126E-01 seconds
```

Although these messages do not terminate a VICTORIA run, in most cases the user should stop the calculation and reduce the time step so that the Courant limit is satisfied.

```
WARNING: relative error in pressure 25.0% exceeds 20% at j= 1, i= 1. Time of occurrence is 1000.0000 seconds
```

This message indicates an error in the thermal-hydraulic input data, as described in Subsection 6.5.3. The error is not severe enough to automatically terminate the calculation, but the user may want to investigate the source of the error and possibly fix the problem.

Problems

The following problem messages can appear in the progress file:

```
CHEMISTRY problem: element Cs in cell 1 in bulk gas region ; attempt number 1
```

This message indicates a mild problem with convergence of the numerical algorithm used to calculate thermochemical equilibrium. This message does not indicate that there should be a mass balance error or other kind of error in the solution.

```
**** element does not exist in VICTORIA... Si
**** species does not exist in VICTORIA...CsOH phase is indicated by a lower case c or g
```

These messages indicate that an element or chemical species that is requested is not in the VICTORIA database. Under some conditions, this message can result in termination of the run.

Information

```
Structure failure temperature exceeded: STOPPING
```

While this is a termination message, it is not considered to be abnormal termination. This message indicates that the user-prescribed structure failure temperature has been attained in a structure for which decay heating is being calculated. Attaining this condition means that a catastrophic failure occurs, possibly resulting in a rapid depressurization of the reactor coolant system. To avoid terminating a calculation in this way, the structure failure temperature should be set to a higher value, as described in Subsection 6.3.6.

```
***** A backup restart file has been saved at step 873, time 873.00 *****
```

This message indicates that the restart file has been updated so that a restart can be done from the indicated value of time.

```
Fuel froths at node j = 1, i = 1 at time = 1000.0000 seconds.
```

This message indicates that the user-prescribed temperature for fuel frothing has been attained.

```
Clad melts with oxide fraction of 0.10000000e+00 at node j = 1, i = 1 at time = 1000.0000 seconds.
```

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This message indicates that the user-prescribed temperature for fuel cladding to melt has been attained.

```
Clad cracks due to oxidation at node j = 1, i = 1 at time = 1000.0000 seconds.
```

This message indicates that the condition for fuel cladding failure due to excess oxidation has been attained.

```
Clad fails at node j = 1, i = 1 at time = 1000.0000 seconds.
```

This message indicates that the user-specified cladding failure temperature has been reached.

```
Reading boundary file      test.bdy  imax in file = 3
```

This message indicates that a file containing data for subdomain coupling is being read.

```
Control rod fails in ring 1, axial level 1 at time = 1000.0000 seconds.
```

This message indicates that the control rods at the prescribed location have failed.

7.3 Graphics File

The binary-formatted graphics file contains more information than the output file. Normally, data are written to this file more frequently than to the output file, so it also contains a better representation of the evolution of predicted values during a run. The exact format of this file is not described here, but the variables that are available for plotting and their dimensions are described.

Data can be extracted from the graphics file in tabular form using EDWARD or plotted using TRAGIC. Usage of EDWARD is described in Subsection 7.3.2. TRAGIC is described in the TRAGIC User's Guide (Masters and Johns, 1993). In the near future, a version of XMGR5 that is able to interpret the VICTORIA graphics file should also be available. XMGR5 is an interactive tool that allows the user to evaluate results quickly.

7.3.1 Plot Variables

Table 7.1 lists the variable names in the order that they appear in the graphics file and gives a brief description and dimensions for each of the variables. The dimensions are as follows: (1) time step, which can have values from 1 to the number of times steps in the calculation; (2) species, which can have values from 1 to 288, the number of species in the VICTORIA database; (3) element, which can have values from 1 to 26, the number of elements in the VICTORIA database; (4) vapor species, which can have values from 1 to 178, the number of vapor species in the VICTORIA database, (5) aerosol species, which can have values from 1 to 110, the number of condensed-phase species in the VICTORIA database; (6) aerosol size, which is the collocation point used to represent aerosol sizes and can have values from 1 to the number of collocation points defined in the input file (maximum of 13); (7) subnode, which can have values from 1 to the number of subnodes representing the fuel, gap, clad, and fuel boundary layer (maximum of 5); (8) fuel subnodes, which can have values from 1 to the number of fuel subn-

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odes defined in the input file (maximum of 2); (9) axial level, j , which can have values from 1 to the number of axial levels defined in the input file (maximum of 30); and (10) radial ring, i , which can have values from 1 to the number of radial rings defined in the input file (maximum of 4). The names and corresponding numerical values for species, element, vapor species, and aerosol species are given in Table 7.2.

Table 7.1: Variables in Graphics File

		Dimensions									
Variable	Description	time step	species	element	vapor species	aerosol species	aerosol size	subnode	fuel subnode	axial level, <i>j</i>	radial ring, <i>i</i>
Time and Volume											
TIME	Time (s)	◆									
VOLUME	Volume (m ³)	◆								◆	◆
Temperatures											
TGAS	Bulk Gas Temperature (K)	◆								◆	◆
TSTRC	Average Structure Temperature (K)	◆								◆	◆
TCEILING	Ceiling Temperature (K)	◆								◆	◆
TWALL	Wall Temperature (K)	◆								◆	◆
TFLOOR	Floor Temperature (K)	◆								◆	◆
TFILM	Temperature of Layer Outside Fuel Cladding (K)	◆								◆	◆
TCLAD	Temperature of Fuel Cladding (K)	◆								◆	◆
TFUEL	Fuel Temperature (K)	◆							◆	◆	◆
Input Gas Pressure											
PRESSURE	Input Bulk Gas Pressure (Pa)	◆								◆	◆
Gas Velocities											
VRGS	Radial Component of Bulk Gas Velocity (m/s)	◆								◆	◆

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Table 7.1: Variables in Graphics File

Variable	Description	Dimensions									
		time step	species	element	vapor species	aerosol species	aerosol size	subnode	fuel subnode	axial level, <i>j</i>	radial ring, <i>i</i>
VZGS	Axial Component of Bulk Gas Velocity (m/s)	◆								◆	◆
Structural Area											
STRCAREA	Structural Surface Area (m ²)	◆								◆	◆
Boundary Layer Thicknesses											
DELSTRC	Boundary Layer Thickness at Structure Surface (m)	◆								◆	◆
DELFUEL	Boundary Layer Thickness at Fuel Surface (m)	◆								◆	◆
Fuel and Control Rod Parameters											
NODEVOL	Volume of Fuel Node (m ³)	◆						◆		◆	◆
CRDVOL	Volume of Boundary Layer at Control Rod Surface (m ³)	◆								◆	◆
ALPHA	Total Fuel Porosity (dimensionless)	◆						◆		◆	◆
GRDIAM	Fuel Grain Diameter (m)	◆							◆	◆	◆
Species Mass Concentrations											
GRAIN	Species Mass Concentration in Grains (kg/m ³)	◆	◆						◆	◆	◆
PORE	Species Mass Concentration in Pores (kg/m ³)	◆	◆					◆		◆	◆
GASDEN	Vapor Species Mass Concentration in Bulk Gas (kg/m ³)	◆			◆					◆	◆
FULFLM	Species Mass Concentration in Fuel Boundary Layer (kg/m ³)	◆	◆							◆	◆
CONTROL	Species Mass Concentration in Control Rod Boundary Layer (kg/m ³)	◆	◆							◆	◆
STRUCT	Species Mass Concentration in Boundary Layer at Structure Surface (kg/m ³)	◆	◆							◆	◆

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Table 7.1: Variables in Graphics File

		Dimensions									
Variable	Description	time step	species	element	vapor species	aerosol species	aerosol size	subnode	fuel subnode	axial level, <i>j</i>	radial ring, <i>i</i>
Mass on Surface											
SPCFLM	Total Mass of Species on Surface (kg)	◆	◆							◆	◆
Gas Properties											
DYNVIS	Dynamic Viscosity of Bulk Gas (Pa·s)	◆								◆	◆
FRPTHM	Mean Free Path in Bulk Gas (m)	◆								◆	◆
GDENSE	Bulk Gas Vapor Density (kg/m ³)	◆								◆	◆
GASK	Thermal Conductivity of Bulk Gas (W/m·K)	◆								◆	◆
Vapor Loss Data											
GASLOST	Vapor Lost as Effluent Through Boundary (kg)	◆			◆						
Aerosol Data											
XMASS	Aerosol Masses at Collocation Points (kg)	◆					◆				
RADIUS	Aerosol Radii at Collocation Points (m)	◆					◆				
AERODEN	Mass Concentration of Aerosol Species (kg/m ³)	◆				◆	◆			◆	◆
CEILING	Aerosol Deposits on Ceiling (kg)	◆				◆				◆	◆
WALL	Aerosol Deposits on Wall (kg)	◆				◆				◆	◆
FLOOR	Aerosol Deposits on Floor (kg)	◆				◆				◆	◆
AMMDAL	Mass Median Diameter of Aerosol (m)	◆								◆	◆
MMD	Mass Median Diameter for Aerosol Species (m)	◆				◆				◆	◆
G50AL	Geometric Mean Diameter of Aerosol (m)	◆								◆	◆
G50	Geometric Mean Diameter for Aerosol Species (m)	◆				◆				◆	◆

Description of VICTORIA Output

Table 7.1: Variables in Graphics File

Variable	Description	Dimensions									
		time step	species	element	vapor species	aerosol species	aerosol size	subnode	fuel subnode	axial level, <i>j</i>	radial ring, <i>i</i>
GEOSDAL	Geometric Standard Deviation of Aerosol (dimensionless)	◆								◆	◆
GEOSD	Geometric Standard Deviation for Aerosol Species (dimensionless)	◆				◆				◆	◆
DEPRAT	Aerosol Mass Deposition Rate (kg/s)	◆				◆				◆	◆
AEROLOST	Aerosol Lost as Effluent Through Boundary (kg)	◆				◆	◆				
SOURCE	Aerosol Source (kg)	◆				◆					
Element Mass Balance Data by Node											
CLGRAIN	Element Mass in Grains (kg)	◆		◆						◆	◆
CLPORE	Element Mass in Pores (kg)	◆		◆						◆	◆
CLGAP	Element Mass in Gap (kg)	◆		◆						◆	◆
CLCLAD	Element Mass In Fuel Cladding (kg)	◆		◆						◆	◆
CLFILM	Element Mass in Fuel Boundary Layer (kg)	◆		◆						◆	◆
CLFILMCR	Element Mass in Control Rod Boundary Layer (kg)	◆		◆						◆	◆
CLGAS	Element Mass in Bulk Gas (kg)	◆		◆						◆	◆
CLAERO	Element Mass in Aerosols (kg)	◆		◆						◆	◆
CLSTRUCT	Element Mass on Structures (kg)	◆		◆						◆	◆
Element Mass Balance Data for Entire Domain											
ELGRAIN	Element Mass in All Fuel Grains (kg)	◆		◆							
ELPORE	Element Mass in All Fuel Pores (kg)	◆		◆							
ELGAP	Element Mass in All Fuel Gaps (kg)	◆		◆							

Description of VICTORIA Output

Table 7.1: Variables in Graphics File

Variable	Description	Dimensions									
		time step	species	element	vapor species	aerosol species	aerosol size	subnode	fuel subnode	axial level, <i>j</i>	radial ring, <i>i</i>
ELCLAD	Element Mass in All Fuel Cladding (kg)	◆		◆							
ELFILM	Element Mass in All Fuel Boundary Layers (kg)	◆		◆							
ELFILMCR	Element Mass in All Control Rod Boundary Layers (kg)	◆		◆							
ELGAS	Element Mass in All Bulk Gas Vapors (kg)	◆		◆							
ELAERO	Element Mass in All Bulk Gas Aerosols (kg)	◆		◆							
ELSTRUCT	Element Mass on All Structures (kg)	◆		◆							
ELOSTGAS	Element Mass Lost as Vapor Effluent Through Boundary (kg)	◆		◆							
ELGASSRC	Element Mass Source as Vapor (kg)	◆		◆							
ELOSTAER	Element Mass Lost as Aerosol Effluent Through Boundary (kg)	◆		◆							
ELAERSRC	Element Mass Source as Aerosol (kg)	◆		◆							
EINITIAL	Initial Element Mass in Domain (kg)	◆		◆							
ELBALANC	Element Mass Balance (kg)	◆		◆							
ELFRBLNC	Element Mass Balance as Fraction of Initial Mass + Mass Source (dimensionless)	◆		◆							
Aerosol Deposition Velocities											
VLAM	Laminar Aerosol Deposition Velocity (m/s)	◆					◆			◆	◆
VTURB	Turbulent Aerosol Deposition Velocity (m/s)	◆					◆			◆	◆
VTHRM	Thermophoretic Aerosol Deposition Velocity (m/s)	◆					◆			◆	◆
VGRAV	Gravitational Settling Velocity of Aerosols (m/s)	◆					◆			◆	◆

Description of VICTORIA Output

Table 7.1: Variables in Graphics File

Variable	Description	Dimensions									
		time step	species	element	vapor species	aerosol species	aerosol size	subnode	fuel subnode	axial level, <i>j</i>	radial ring, <i>i</i>
AVLAM	Average Laminar Aerosol Deposition Velocity (m/s)	◆								◆	◆
AVTURB	Average Turbulent Aerosol Deposition Velocity (m/s)	◆								◆	◆
AVTHRM	Average Thermophoretic Aerosol Deposition Velocity (m/s)	◆								◆	◆
AVGRAV	Average Gravitational Settling Velocity of Aerosols (m/s)	◆								◆	◆
VIRREG	Aerosol Deposition Velocity from Flow Irregularities (m/s)	◆					◆			◆	◆
AVIRREG	Average Aerosol Deposition Velocity from Flow Irregularities (m/s)	◆								◆	◆
CPU Time Data											
CPUFUL	CPU Time for Fission Product Release (s)	◆									
CPUCHM	CPU Time for Chemistry (s)	◆									
CPUGTR	CPU Time for Gas Transport (s)	◆									
CPUARO	CPU Time for Aerosol Agglomeration and Deposition (s)	◆									
CPUDCA	CPU Time for Decay Heating (s)	◆									
CPUATR	CPU Time for Aerosol Transport (s)	◆									
CPUBDL	CPU Time for Boundary Layer Diffusion (s)	◆									
Deposition Data											
SCNDNS	Element Mass Condensed in Structure Boundary Layer (kg)	◆		◆						◆	◆
SDEPOS	Element Mass Deposited in Structure Boundary Layer (kg)	◆		◆						◆	◆

Description of VICTORIA Output

Table 7.1: Variables in Graphics File

Variable	Description	Dimensions									
		time step	species	element	vapor species	aerosol species	aerosol size	subnode	fuel subnode	axial level, <i>j</i>	radial ring, <i>i</i>
SVAPOR	Element Mass as Vapor in Structure Boundary Layer (kg)	◆		◆						◆	◆
Decay Power Data											
GDPOW	Decay Power in Bulk Gas (W/m ³)	◆								◆	◆
SDPOW	Decay Power on Structures (W/m ²)	◆								◆	◆
Calculated Gas Pressures											
PFUEL	Total Gas Pressure in Fuel (Pa)	◆							◆	◆	◆
PGAP	Total Gas Pressure in Fuel/Clad Gap (Pa)	◆								◆	◆
PCLAD	Total Gas Pressure in Fuel Cladding (Pa)	◆								◆	◆
PFILM	Total Gas Pressure in Fuel Boundary Layer (Pa)	◆								◆	◆
PCROD	Total Gas Pressure In Control Rod Boundary Layer (Pa)	◆								◆	◆
PGAS	Total Gas Pressure in Bulk Gas (Pa)	◆								◆	◆
PSTRC	Total Gas Pressure in Structure Boundary Layer (Pa)	◆								◆	◆
Release from Fuel											
FRLSE	Fractional Fission Product Release from Fuel (dimensionless)	◆		◆							

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Table 7.2: Species Names and Numbers in Graphics File

Chemical Symbol	Species		Element		Vapor Species		Aerosol Species	
	Name	No.	Name	No.	Name	No.	Name	No.
CsI(c)	CsIc	1					CsIa	1
CsI(g)	CsIg	2			CsIv	1		
CsOH(c)	CsOHc	3					CsOHa	2
CsOH(g)	CsOHg	4			CsOHv	2		
Cs(g)	Csg	5	Cs	2	Csv	3		
Cs ₂ O(g)	Cs ₂ Og	6			Cs ₂ Ov	4		
Cs ₂ (OH) ₂ (g)	Cs ₂ O ₂ H ₂ g	7			Cs ₂ O ₂ H ₂ v	5		
Cs(c)	Csc	8					Csa	3
Cs ₂ O(c)	Cs ₂ Oc	9					Cs ₂ Oa	4
Cs ₂ UO ₄ (c)	Cs ₂ UO ₄ c	10					Cs ₂ UO ₄ a	5
Cs ₂ U ₂ O ₇ (c)	Cs ₂ U ₂ O ₇ c	11					Cs ₂ U ₂ O ₇ a	6
Cs ₂ MoO ₄ (c)	Cs ₂ MoO ₄ c	12					Cs ₂ MoO ₄ a	7
BaOH(g)	BaOHg	13			BaOHv	6		
Ba(OH) ₂ (g)	BaO ₂ H ₂ g	14			BaO ₂ H ₂ v	7		
Ba(OH) ₂ (c)	BaO ₂ H ₂ c	15					BaO ₂ H ₂ a	8
BaO(g)	BaOg	16			BaOv	8		
BaO(c)	BaOc	17					BaOa	9
BaI(g)	BaIg	18			BaIv	9		
BaI ₂ (g)	BaI ₂ g	19			BaI ₂ v	10		
BaI ₂ (c)	BaI ₂ c	20					BaI ₂ a	10
Ba(g)	Bag	21	Ba	1	Bav	11		
Ba(c)	Bac	22					Baa	11
BaTe(c)	BaTec	23					BaTea	12
BaZrO ₃ (c)	BaZrO ₃ c	24					BaZrO ₃ a	13
BaUO ₄ (c)	BaUO ₄ c	25					BaUO ₄ a	14

Description of VICTORIA Output

Table 7.2: Species Names and Numbers in Graphics File

Chemical Symbol	Species		Element		Vapor Species		Aerosol Species	
	Name	No.	Name	No.	Name	No.	Name	No.
BaMoO ₄ (c)	BaMoO4c	26					BaMoO4a	15
I(g)	Ig	27	I	4	Iv	12		
I ₂ (g)	I2g	28			I2v	13		
HI(g)	HIg	29			HIv	14		
H(g)	Hg	30	H	3	Hv	15		
H ₂ (g)	H2g	31			H2v	16		
H ₂ O(g)	H2Og	32			H2Ov	17		
SrOH(g)	SrOHg	33			SrOHv	18		
Sr(OH) ₂ (c)	SrO2H2c	34					SrO2H2a	16
Sr(OH) ₂ (g)	SrO2H2g	35			SrO2H2v	19		
SrO(c)	SrOc	36					SrOa	17
SrO(g)	SrOg	37			SrOv	20		
SrI(g)	SrIg	38			SrIv	21		
SrI ₂ (g)	SrI2g	39			SrI2v	22		
SrI ₂ (c)	SrI2c	40					SrI2a	18
Sr(g)	Srg	41	Sr	9	Srv	23		
Sr(c)	Src	42					Sra	19
SrUO ₄ (c)	SrUO4c	43					SrUO4a	20
SrZrO ₃ (c)	SrZrO3c	44					SrZrO3a	21
SrMoO ₄ (c)	SrMoO4c	45					SrMoO4a	22
ZrO(g)	ZrOg	46			ZrOv	24		
ZrO ₂ (g)	ZrO2g	47			ZrO2v	25		
ZrO ₂ (c)	ZrO2c	48					ZrO2a	23
Zr(g)	Zrg	49	Zr	12	Zrv	26		
Zr(c)	Zrc	50					Zra	24
Sn(c)	Snc	51					Sna	25
Sn(g)	Sng	52	Sn	8	Snv	27		

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Table 7.2: Species Names and Numbers in Graphics File

Chemical Symbol	Species		Element		Vapor Species		Aerosol Species	
	Name	No.	Name	No.	Name	No.	Name	No.
SnO(g)	SnOg	53			SnOv	28		
SnO(c)	SnOc	54					SnOa	26
SnO ₂ (c)	SnO2c	55					SnO2a	27
SnO ₂ (g)	SnO2g	56			SnO2v	29		
SnI ₂ (g)	SnI2g	57			SnI2v	30		
SnI ₂ (c)	SnI2c	58					SnI2a	28
SnTe(g)	SnTeg	59			SnTev	31		
SnTe(c)	SnTec	60					SnTea	29
SnH ₄ (g)	SnH4g	61			SnH4v	32		
Te(g)	Teg	62	Te	10	Tev	33		
Te(c)	Tec	63					Tea	30
Te ₂ (g)	Te2g	64			Te2v	34		
TeO(g)	TeOg	65			TeOv	35		
TeO ₂ (g)	TeO2g	66			TeO2v	36		
TeO ₂ (c)	TeO2c	67					TeO2a	31
Te ₂ O ₂ (g)	Te2O2g	68			Te2O2v	37		
H ₂ Te(g)	H2Teg	69			H2Tev	38		
UO ₂ (c)	UO2c	70					UO2a	32
UO ₂ (g)	UO2g	71			UO2v	39		
U(c)	Uc	72					Ua	33
U(g)	Ug	73	U	11	Uv	40		
U ₄ O ₉ (c)	U4O9c	74					U4O9a	34
U ₃ O ₈ (c)	U3O8c	75					U3O8a	35
UO ₃ (c)	UO3c	76					UO3a	36
Kr(g)	Krg	77	Kr	23	Krv	41		
Xe(g)	Xeg	78	Xe	24	Xev	42		
O ₂ (g)	O2g	79			O2v	43		

Description of VICTORIA Output

Table 7.2: Species Names and Numbers in Graphics File

Chemical Symbol	Species		Element		Vapor Species		Aerosol Species	
	Name	No.	Name	No.	Name	No.	Name	No.
O(g)	Og	80	O	6	Ov	44		
Fe(c)	Fec	81					Fea	37
Fe(g)	Feg	82	Fe	14	Fev	45		
FeO(c)	FeOc	83					FeOa	38
FeO(g)	FeOg	84			FeOv	46		
Fe ₂ O ₃ (c)	Fe2O3c	85					Fe2O3a	39
Fe ₃ O ₄ (c)	Fe3O4c	86					Fe3O4a	40
FeI ₂ (c)	FeI2c	87					FeI2a	41
FeI ₂ (g)	FeI2g	88			FeI2v	47		
Fe ₂ I ₄ (g)	Fe2I4g	89			Fe2I4v	48		
FeTe(c)	FeTec	90					FeTea	42
FeTe ₂ (c)	FeTe2c	91					FeTe2a	43
Mo(c)	Moc	92					Moa	44
Mo(g)	Mog	93	Mo	5	Mov	49		
MoO(g)	MoOg	94			MoOv	50		
MoO ₂ (c)	MoO2c	95					MoO2a	45
MoO ₂ (g)	MoO2g	96			MoO2v	51		
MoO ₃ (c)	MoO3c	97					MoO3a	46
MoO ₃ (g)	MoO3g	98			MoO3v	52		
Ag(g)	Agg	99	Ag	18	Agv	53		
Ag(c)	Agc	100					Aga	47
AgTe(g)	AgTeg	101			AgTev	54		
Ag ₂ Te(c)	Ag2Tec	102					Ag2Tea	48
B(c)	Bc	103					Bae	49
B(g)	Bg	104	B	13	Bv	55		
BI(g)	BIg	105			BIv	56		
BI ₂ (g)	BI2g	106			BI2v	57		

Description of VICTORIA Output

Table 7.2: Species Names and Numbers in Graphics File

Chemical Symbol	Species		Element		Vapor Species		Aerosol Species	
	Name	No.	Name	No.	Name	No.	Name	No.
BI ₃ (g)	BI3g	107			BI3v	58		
BO(g)	BOg	108			BOv	59		
BO ₂ (g)	BO2g	109			BO2v	60		
B ₂ O ₃ (c)	B2O3c	110					B2O3a	50
B ₂ O ₃ (g)	B2O3g	111			B2O3v	61		
BTe(g)	BTEg	112			BTEv	62		
CsBO ₂ (c)	CsBO2c	113					CsBO2a	51
HBO ₂ (c)	HBO2c	114					HBO2a	52
HBO ₂ (g)	HBO2g	115			HBO2v	63		
H ₃ BO ₃ (c)	H3BO3c	116					H3BO3a	53
H ₃ BO ₃ (g)	H3BO3g	117			H3BO3v	64		
ZrB ₂ (c)	ZrB2c	118					ZrB2a	54
Cd(g)	Cdg	119	Cd	20	Cdv	65		
Cd(c)	Cdc	120					Cda	55
CdO(c)	CdOc	121					CdOa	56
CdO(g)	CdOg	122			CdOv	66		
CdTe(c)	CdTec	123					CdTea	57
CdTe(g)	CdTeg	124			CdTev	67		
Cr(g)	Crg	125	Cr	15	Crv	68		
Cr(c)	Crc	126					Cra	58
Cr ₂ O ₃ (c)	Cr2O3c	127					Cr2O3a	59
CrTe(c)	CrTec	128					CrTea	60
In(g)	Ing	129	In	19	Inv	69		
In(c)	Inc	130					Ina	61
In ₂ O ₃ (c)	In2O3c	131					In2O3a	62
InTe(c)	InTec	132					InTea	63
InTe(g)	InTeg	133			InTev	70		

Description of VICTORIA Output

Table 7.2: Species Names and Numbers in Graphics File

Chemical Symbol	Species		Element		Vapor Species		Aerosol Species	
	Name	No.	Name	No.	Name	No.	Name	No.
InOH(g)	InOHg	134			InOHv	71		
Mn(g)	Mng	135	Mn	16	Mnv	72		
Mn(c)	Mnc	136					Mna	64
MnO(c)	MnOc	137					MnOa	65
Mn ₃ O ₄ (c)	Mn3O4c	138					Mn3O4a	66
MnTe(c)	MnTec	139					MnTea	67
MnTe ₂ (c)	MnTe2c	140					MnTe2a	68
Ni(g)	Nig	141	Ni	17	Niv	73		
Ni(c)	Nic	142					Nia	69
NiO(c)	NiOc	143					NiOa	70
Ru(g)	Rug	144	Ru	7	Ruv	74		
Ru(c)	Ruc	145					Rua	71
RuO ₂ (c)	RuO2c	146					RuO2a	72
RuO ₃ (g)	RuO3g	147			RuO3v	75		
RuO ₄ (g)	RuO4g	148			RuO4v	76		
Sb(g)	Sbg	149	Sb	21	Sbv	77		
Sb(c)	Sbc	150					Sba	73
Sb ₂ (g)	Sb2g	151			Sb2v	78		
Sb ₄ (g)	Sb4g	152			Sb4v	78		
Sb ₂ O ₃ (c)	Sb2O3c	153					Sb2O3a	74
SbTe(g)	SbTeg	154			SbTev	80		
Sb ₂ Te ₃ (c)	Sb2Te3c	155					Sb2Te3a	75
Eu(g)	Eug	156	Eu	22	Euv	81		
Eu(c)	Euc	157					Eua	76
EuO(g)	EuOg	158			EuOv	82		
EuO(c)	EuOc	159					EuOa	77
Eu ₂ O ₃ (c)	Eu2O3c	160					Eu2O3a	78

Description of VICTORIA Output

Table 7.2: Species Names and Numbers in Graphics File

Chemical Symbol	Species		Element		Vapor Species		Aerosol Species	
	Name	No.	Name	No.	Name	No.	Name	No.
EuTe(g)	EuTeg	161			EuTev	83		
ZrH(g)	ZrHg	162			ZrHv	84		
Sn ₂ Te ₂ (g)	Sn2Te2g	163			Sn2Te2v	85		
H ₂ MoO ₄ (g)	H2MoO4g	164			H2MoO4v	86		
He(g)	Heg	165			Hev	87		
CsO(g)	CsOg	166			CsOv	88		
Cs ₂ (g)	Cs2g	167			Cs2v	89		
CsH(g)	CsHg	168			CsHv	90		
CsBO ₂ (g)	CsBO2g	169			CsBO2v	91		
Cs ₂ U ₄ O ₁₂ (c)	Cs2U4O12	170					Cs2U4O1a	79
Cs ₂ ZrO ₃ (c)	Cs2ZrO3c	171					Cs2ZrO3a	80
Cs ₂ Zr ₂ O ₅ (c)	Cs2Zr2O5	172					Cs2Zr2Oa	81
Cs ₂ Zr ₃ O ₇ (c)	Cs2Zr3O7	173					Cs2Zr3Oa	82
Cs ₂ Te(c)	Cs2Tec	174					Cs2Tea	83
Cs ₂ TeO ₃ (c)	Cs2TeO3c	175					Cs2TeO3a	84
Cs ₂ Te ₂ O ₅ (c)	Cs2Te2O5	176					Cs2Te2Oa	85
Cs ₂ Te ₄ O ₉ (c)	Cs2Te4O9	177					Cs2Te4Oa	86
Cs ₂ TeO ₄ (c)	Cs2TeO4c	178					Cs2TeO4a	87
Cs ₂ Te ₄ O ₁₂ (c)	Cs2Te4O1	179					Cs2Te4Oa	88
Cs ₂ O ₂ (g)	Cs2O2g	180			Cs2O2v	92		
Cs ₂ I ₂ (g)	Cs2I2g	181			Cs2I2v	93		
Cs ₂ CrO ₄ (g)	Cs2CrO4g	182			Cs2CrO4v	94		
Cs ₂ MoO ₄ (g)	Cs2MoO4g	183			Cs2MoO4v	95		
Cs ₂ Cr ₂ O ₇ (c)	Cs2Cr2O7	184					Cs2Cr2Oa	89
Cs ₂ CrO ₄ (c)	Cs2CrO4c	185					Cs2CrO4a	90
Cs ₃ CrO ₄ (c)	Cs3CrO4c	186					Cs3CrO4a	91
Cs ₄ CrO ₄ (c)	Cs4CrO4c	187					Cs4CrO4a	92

Description of VICTORIA Output

Table 7.2: Species Names and Numbers in Graphics File

Chemical Symbol	Species		Element		Vapor Species		Aerosol Species	
	Name	No.	Name	No.	Name	No.	Name	No.
IO(g)	IOg	188			IOv	96		
HO(g)	HOg	189			HOv	97		
HIO(g)	HIOg	190			HIOv	98		
BaH(g)	BaHg	191			BaHv	99		
Ba ₂ O(g)	Ba2Og	192			Ba2Ov	100		
BaH ₂ (c)	BaH2c	193					BaH2a	93
Ba ₂ (g)	Ba2g	194			Ba2v	101		
Ba ₂ O ₂ (g)	Ba2O2g	195			Ba2O2v	102		
BaMoO ₄ (g)	BaMoO4g	196			BaMoO4v	103		
SrH ₂ (c)	SrH2c	197					SrH2a	94
Sr ₂ (g)	Sr2g	198			Sr2v	104		
ZrI ₄ (c)	ZrI4c	199					ZrI4a	95
ZrTe ₂ (c)	ZrTe2c	200					ZrTe2a	96
ZrI ₄ (g)	ZrI4g	201			ZrI4v	105		
ZrI ₃ (g)	ZrI3g	202			ZrI3v	106		
ZrI ₂ (g)	ZrI2g	203			ZrI2v	107		
ZrI(g)	ZrIg	204			ZrIv	108		
ZrOH(g)	ZrOHg	205			ZrOHv	109		
Zr(OH) ₂ (g)	ZrH2O2g	206			ZrH2O2v	110		
SnOH(g)	SnOHg	207			SnOHv	111		
Sn(OH) ₂ (g)	SnH2O2g	208			SnH2O2v	112		
Sn ₂ (g)	Sn2g	209			Sn2v	113		
SnTe ₂ (g)	SnTe2g	210			SnTe2v	114		
H ₂ TeO ₃ (g)	TeO3H2g	211			TeO3H2v	115		
Tel ₄ (g)	Tel4g	212			Tel4v	116		
TeOI ₂ (g)	TeOI2g	213			TeOI2v	117		
Tel ₄ (c)	Tel4c	214					Tel4a	97

Description of VICTORIA Output

Table 7.2: Species Names and Numbers in Graphics File

Chemical Symbol	Species		Element		Vapor Species		Aerosol Species	
	Name	No.	Name	No.	Name	No.	Name	No.
H ₂ TeO ₄ (c)	TeH2O4c	215					TeH2O4a	98
TeOH(g)	TeOHg	216			TeOHv	118		
Te(OH) ₂ (g)	TeH2O2g	217			TeH2O2v	119		
H ₄ UO ₅ (c)	UH4O5c	218					UH4O5a	99
UO(g)	UOg	219			UOv	120		
UO ₃ (g)	UO3g	220			UO3v	121		
UOH(g)	UOHg	221			UOHv	122		
U(OH) ₂ (g)	UH2O2g	222			UH2O2v	123		
FeOH(g)	FeOHg	223			FeOHv	124		
Fe(OH) ₂ (g)	FeO2H2g	224			FeO2H2v	125		
Fe(OH) ₂ (c)	FeO2H2c	225					FeO2H2a	100
Mol ₄ (c)	Mol4c	226					Mol4a	101
Mol ₃ (c)	Mol3c	227					Mol3a	102
Mol ₂ (c)	Mol2c	228					Mol2a	103
Mo ₂ (g)	Mo2g	229			Mo2v	126		
Mo ₂ O ₆ (g)	Mo2O6g	230			Mo2O6v	127		
MoOH(g)	MoOHg	231			MoOHv	128		
Mo(OH) ₂ (g)	MoH2O2g	232			MoH2O2v	129		
In ₂ O(g)	In2Og	233			In2Ov	130		
Mol(g)	Molg	234			Molv	131		
Mol ₂ (g)	Mol2g	235			Mol2v	132		
Mol ₃ (g)	Mol3g	236			Mol3v	133		
MoO ₂ l ₂ (g)	MoO2l2g	237			MoO2l2v	134		
Mo ₃ O ₉ (g)	Mo3O9g	238			Mo3O9v	135		
Mo ₄ O ₁₂ (g)	Mo4O12g	239			Mo4O12v	136		
Mo5O15(g)	Mo5O15g	240			Mo5O15v	137		
Mol ₄ (g)	Mol4g	241			Mol4v	138		

Description of VICTORIA Output

Table 7.2: Species Names and Numbers in Graphics File

Chemical Symbol	Species		Element		Vapor Species		Aerosol Species	
	Name	No.	Name	No.	Name	No.	Name	No.
AgI(c)	AgIc	242					AgIa	104
AgI(g)	AgIg	243			AgIv	139		
AgOH(g)	AgOHg	244			AgOHv	140		
Ag(OH) ₂ (g)	AgH ₂ O ₂ g	245			AgH ₂ O ₂ v	141		
B ₂ (g)	B ₂ g	246			B ₂ v	142		
BOH(g)	BOHg	247			BOHv	143		
BH(g)	BHg	248			BHv	144		
BH ₂ (g)	BH ₂ g	249			BH ₂ v	145		
BH ₃ (g)	BH ₃ g	250			BH ₃ v	146		
B ₂ H ₆ (g)	B ₂ H ₆ g	251			B ₂ H ₆ v	147		
B(OH) ₂ (g)	BH ₂ O ₂ g	252			BH ₂ O ₂ v	148		
CdOH(g)	CdOHg	253			CdOHv	149		
Cd(OH) ₂ (g)	CdH ₂ O ₂ g	254			CdH ₂ O ₂ v	150		
CdI(g)	CdIg	255			CdIv	151		
CdI ₂ (c)	CdI ₂ c	256					CdI ₂ a	105
CdI ₂ (g)	CdI ₂ g	257			CdI ₂ v	152		
CrOH(g)	CrOHg	258			CrOHv	153		
Cr(OH) ₂ (g)	CrH ₂ O ₂ g	259			CrH ₂ O ₂ v	154		
CrO(g)	CrOg	260			CrOv	155		
CrO ₂ (g)	CrO ₂ g	261			CrO ₂ v	156		
CrO ₃ (g)	CrO ₃ g	262			CrO ₃ v	157		
CrI(g)	CrIg	263			CrIv	158		
CrI ₂ (c)	CrI ₂ c	264					CrI ₂ a	106
CrI ₂ (g)	CrI ₂ g	265			CrI ₂ v	159		
InI(c)	InIc	266					InIa	107
InI(g)	InIg	267			InIv	160		
In(OH) ₂ (g)	InH ₂ O ₂ g	268			InH ₂ O ₂ v	161		

Description of VICTORIA Output

Table 7.2: Species Names and Numbers in Graphics File

Chemical Symbol	Species		Element		Vapor Species		Aerosol Species	
	Name	No.	Name	No.	Name	No.	Name	No.
MnO(g)	MnOg	269			MnOv	162		
MnOH(g)	MnOHg	270			MnOHv	163		
NiO(g)	NiOg	271			NiOv	164		
NiOH(g)	NiOHg	272			NiOHv	165		
Ni(OH) ₂ (g)	NiH2O2g	273			NiH2O2v	166		
NiI ₂ (c)	NiI2c	274					NiI2a	108
Ru ₃ U(c)	Ru3Uc	275					Ru3Ua	109
RuTe ₂ (c)	RuTe2c	276					RuTe2a	110
RuO ₂ (g)	RuO2g	277			RuO2v	167		
RuO(g)	RuOg	278			RuOv	168		
RuOH(g)	RuOHg	279			RuOHv	169		
Ru(OH) ₂ (g)	RuH2O2g	280			RuH2O2v	170		
SbOH(g)	SbOHg	281			SbOHv	171		
Sb(OH) ₂ (g)	SbH2O2g	282			SbH2O2v	172		
SbH ₃ (g)	SbH3g	283			SbH3v	173		
EuOH(g)	EuOHg	284			EuOHv	174		
Eu(OH) ₂ (g)	EuH2O2g	285			EuH2O2v	175		
Eu ₂ O(g)	Eu2Og	286			Eu2Ov	176		
Eu ₂ O ₂ (g)	Eu2O2g	287			Eu2O2v	177		
Ar(g)	Arg	288	Ar	26	Arv	178		

As a rule, all species names end with either a *c* (for condensed phase) or a *g* (for gaseous phase); however, there are several exceptions where the species name exceeds 8 characters, which is the maximum permitted by the TRAGIC code. These species names are truncated to 8 characters. All vapor species names end with a *v*.

As a rule, aerosol species names end with an *a*; however, like the species names, some of the aerosol names are truncated to 8 characters. The user should exercise some care

Description of VICTORIA Output

in using the correct nomenclature for variables, depending on whether they are species, vapor species, or aerosol species. TRAGIC accepts either the variable name or number; EDWARD accepts only the variable name.

Species names with suffix *a* or *v* are only used in the graphics file; VICTORIA input and output files use only the *c* and *g* suffixes to designate the phase.

7.3.2 Using EDWARD

EDWARD is a program that extracts user-specified data from the VICTORIA unformatted graphics file. It generates an ASCII file that is readable by most plotting packages. It is particularly useful when publication-quality plots are needed.

User input to EDWARD consists of the names of the graphics file and the EDWARD output file, each contained in single quotes, followed by a set of lines describing the variables to be extracted. Comment lines can be included as desired by placing a *\$* in the first position of the line. A complete input file would look like the following:

```
$
$ Sample EDWARD input file
$
$ Names of VICTORIA-92 graphics dump and EDWARD output file
$   'sample.grf' 'edward.out'
$
$ Volume of cell j=5, i=1
$   VOLUME 5 1
$
$ Bulk gas density of CsI vapor, cell j=5, i=1
$   GASDEN CsIg 5 1
$
$ Aerosol density of CsI aerosol, collocation point=2, cell j=5, i=1
$   AERODEN CsIc 2 5 1
$
$ Ceiling, wall, floor deposition of CsI aerosol, cell j=5, i=1
$   CEILING CsIc 5 1
$   WALL CsIc 5 1
$   FLOOR CsIc 5 1
$
```

This input file directs EDWARD to read from a graphics file named *sample.grf*. The output from EDWARD is written to the file named *edward.out*. Variable and species names can be in upper, lower, or mixed case. Subscripts for each variable must correspond exactly to the dimensions that are required for each variable, as listed in Table 7.1, with one exception; no value for *time step* can be specified because data are tabulated by EDWARD for each value of time that is stored in the graphics file. The EDWARD input file should always be named *edward.inp*.

The command to start EDWARD is simply

```
% edwd
```

For this command to be successful, *edwd* must be in the user's path and *edward.inp* must be in the current working directory and *sample.grf* must be in the location specified in *edward.inp*. The output file created, *edward.out*, has the following format:

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```
$
$ Victoria 2.0 1 Jul 1997
$ pid19063
$ Thermal Gradient Tube
$ Thu Feb 18 13:23:52 1993
$ Graphics dump = sample.grf
$ EDWARD output = edward.out
$
$ VOLUME      ( 5, 1)
$ GASDEN CsIg ( 2, 5, 1)
$ AERODEN CsIc ( 1, 2, 5, 1)
$ CEILING CsIc ( 1, 5, 1)
$ WALL CsIc ( 1, 5, 1)
$ FLOOR CsIc ( 1, 5, 1)
1.0000E+00 1.4043E-02 5.2665E-06 1.2018E-18 0.0000E+00 2.1723E-17 0.0000E+00
5.0000E+00 1.4043E-02 5.2666E-06 4.1867E-18 0.0000E+00 1.0862E-16 0.0000E+00
1.0000E+01 1.4043E-02 5.2686E-06 5.7301E-18 0.0000E+00 2.1725E-16 0.0000E+00
1.5000E+01 1.4043E-02 5.2722E-06 6.3078E-18 0.0000E+00 3.2595E-16 0.0000E+00
2.0000E+01 1.4043E-02 5.2761E-06 6.5303E-18 0.0000E+00 4.3472E-16 0.0000E+00
2.5000E+01 1.4043E-02 5.2794E-06 6.6200E-18 0.0000E+00 5.4357E-16 0.0000E+00
3.0000E+01 1.4043E-02 5.2816E-06 6.6583E-18 0.0000E+00 6.5247E-16 0.0000E+00
3.5000E+01 1.4043E-02 5.2830E-06 6.6756E-18 0.0000E+00 7.6142E-16 0.0000E+00
4.0000E+01 1.4043E-02 5.2837E-06 6.6837E-18 0.0000E+00 8.7038E-16 0.0000E+00
4.5000E+01 1.4043E-02 5.2841E-06 6.6876E-18 0.0000E+00 9.7936E-16 0.0000E+00
5.0000E+01 1.4043E-02 5.2843E-06 6.6894E-18 0.0000E+00 1.0883E-15 0.0000E+00
```

The first eight lines of output describe the version of VICTORIA that created the graphics file, the process ID of the run that generated the graphics file, the name of the calculation, the date on which the graphics file was created, the name of the graphics file, and the name of the EDWARD output file. The next six lines echo the plot variables that were requested in the `edward.inp` file. Finally, the requested data are tabulated. The first variable in the table is always time. The other variables are in the same order in which they are listed, which is the same order in which they appear in the EDWARD input file.

7.4 Error Message File

When a VICTORIA run completes successfully, the error message file should look like the following:

```
STOP: END OF CALCULATION
Note: IEEE floating-point exception flags raised:
      Inexact; Underflow;
IEEE floating-point exception traps enabled:
      overflow; division by zero; invalid operation;
Nonstandard floating-point mode enabled
See the Numerical Computation Guide, ieee_flags(3M), ieee_handler(3M),
ieee_sun(3M)
18894.0u 217.0s 10:41:22 49% 0+0k 0+0io 0pf+0w
```

However, if an error occurs at the operating system level, either because of an illegal operation within the VICTORIA code or because of an external interruption to the run (e.g., the user killing the process), a message describing why the run was terminated will usually appear in this file. An exception is when a power or other failure results in a sudden system crash, preventing the computer from shutting down gracefully.

Description of VICTORIA Output

Part III: Thermochemical and Thermophysical Databases

8.0 Thermochemical and Physical Data

8.1 Element Data

Element data, including atomic weight, grain lattice diffusion coefficients, boiling point, and density at boiling point, are listed in Table 8.1. Default grain lattice diffusion coefficients, $D_G(i) = D_0(i) \cdot \exp(-\theta(i)/T)$, for most of the elements (i) are Matzke's recommended values for the volatile elements (1986). These default values can be modified by input data, as described in Chapter 6. Melting point, boiling point, and density data are from Emsley (1992).

Table 8.1: Element Data Used in VICTORIA

Element		Atomic Weight (kg/kg-mol)	Default Grain Lattice Diffusion Coefficients		Melting Point (K)	Boiling Point (K)	Density (kg/m ³)
Number	Symbol		$D_0(i)$ (m ² /s)	$\theta(i)$ (K)			
1	Ba	137.3	$5 \cdot 10^{-5}$	$5 \cdot 10^4$	1002	1910	3325 ^a
2	Cs	132.9	$5 \cdot 10^{-5}$	$5 \cdot 10^4$	302	952	1843 ^a
3	H	1.0	0	$5 \cdot 10^4$	14	20	71 ^b
4	I	126.9	$5 \cdot 10^{-5}$	$5 \cdot 10^4$	387	458	4930 ^c
5	Mo	95.9	$5 \cdot 10^{-5}$	$5 \cdot 10^4$	2890	4885	9330 ^a
6	O	16.0	0	$5 \cdot 10^4$	55	90	1140 ^b
7	Ru	101.1	$5 \cdot 10^{-5}$	$5 \cdot 10^4$	2583	4173	10900 ^a
8	Sn	118.7	$5 \cdot 10^{-5}$	$5 \cdot 10^4$	505	2543	6973 ^a
9	Sr	87.6	$5 \cdot 10^{-5}$	$5 \cdot 10^4$	1042	1657	2375 ^a
10	Te	127.6	$5 \cdot 10^{-5}$	$5 \cdot 10^4$	723	1263	5797 ^a
11	U	238.0	0	$5 \cdot 10^4$	1406	4018	17907 ^a
12	Zr	91.2	$5 \cdot 10^{-5}$	$5 \cdot 10^4$	2125	4650	5800 ^a
13	B	10.8	0	$5 \cdot 10^4$	2573	3931	2340 ^c
14	Fe	55.8	0	$5 \cdot 10^4$	1808	3023	7035 ^a
15	Cr	52.0	0	$5 \cdot 10^4$	2130	2945	6460 ^a
16	Mn	54.9	0	$5 \cdot 10^4$	1517	2235	6430 ^a

Thermochemical and Physical Data

Table 8.1: Element Data Used in VICTORIA

Element		Atomic Weight (kg/kg-mol)	Default Grain Lattice Diffusion Coefficients		Melting Point (K)	Boiling Point (K)	Density (kg/m ³)
Number	Symbol		$D_0(i)$ (m ² /s)	$\theta(i)$ (K)			
17	Ni	58.7	0	$5 \cdot 10^4$	1726	3005	7780 ^a
18	Ag	107.9	0	$5 \cdot 10^4$	1235	2485	9345 ^a
19	In	114.8	0	$5 \cdot 10^4$	429	2353	7032 ^a
20	Cd	112.4	0	$5 \cdot 10^4$	594	1038	7996 ^a
21	Sb	121.8	$5 \cdot 10^{-5}$	$5 \cdot 10^4$	904	1908	6483 ^a
22	Eu	152.0	$5 \cdot 10^{-5}$	$5 \cdot 10^4$	1095	1870	5243 ^b
23	Kr	83.8	$5 \cdot 10^{-5}$	$5 \cdot 10^4$	117	121	2413 ^c
24	Xe	131.3	$5 \cdot 10^{-5}$	$5 \cdot 10^4$	161	166	2939 ^c
25	He	4.0	0	$5 \cdot 10^4$	0.95	4.2	125 ^c
26	Ar	39.9	0	$5 \cdot 10^4$	84	87	1380 ^c

a. Density of liquid at melting point.

b. Density of liquid at room temperature.

c. Density of liquid at boiling point.

8.2 Fission Product Decay Power Data

Decay power data are taken from Ostmeyer (1984). There are eleven elements for which decay powers are calculated, as shown in Table 8.2. The logarithms of the decay power data given in Table 8.2 are interpolated linearly between the values of time listed.

Some of the data in Table 8.2 appear to be in error because they do not decrease monotonically with time; however, the evolution of decay power is more complex than one might at first expect because these data account for multiple isotopes and for the power generated by daughter elements. The overall power accounted for by the elements in Table 8.2 immediately after shutdown represents 2.743% of the reactor power just before shutdown. The total decay heat, calculated from the data in Table 8.2, as a function of time after reactor shutdown, is plotted in Figure 8.1.

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Table 8.2: Decay Power Data Used in VICTORIA

	Decay Power for a Fission Product per Unit Reactor Power Prior to Shutdown (W/kW)										
Time (s)	Ba	Cs	I	Mo	Ru	Sr	Te	U	Sb	Kr	Xe
0	2.60	4.40	4.70	1.90	0.53	3.40	2.10	1.20	1.80	2.40	2.40
6	2.20	3.20	4.10	2.10	0.53	2.60	1.80	1.20	1.60	1.90	2.10
12	2.00	3.20	4.10	2.10	0.56	2.40	1.70	1.20	1.60	1.70	1.90
18	1.80	2.90	3.80	2.10	0.56	2.30	1.60	1.20	1.50	1.60	1.80
30	1.60	2.80	3.50	2.00	0.59	2.10	1.40	1.20	1.50	1.50	1.70
60	1.40	2.30	3.30	1.80	0.59	1.80	1.30	1.20	1.40	1.30	1.50
120	1.30	1.90	2.90	1.50	0.56	1.50	1.20	1.20	1.20	1.10	1.20
240	1.20	1.60	2.80	1.20	0.50	1.30	1.10	1.10	1.00	0.97	0.94
600	1.00	1.20	2.60	0.85	0.44	1.10	1.10	0.91	0.67	0.79	0.70
1200	0.79	0.91	2.40	0.61	0.38	0.88	1.00	0.70	0.50	0.76	0.53
3600	0.47	0.38	1.90	0.25	0.35	0.76	0.85	0.22	0.26	0.70	0.29
5400	0.38	0.23	1.60	0.19	0.35	0.73	0.79	0.10	0.18	0.62	0.20
7200	0.35	0.15	1.50	0.17	0.32	0.70	0.76	0.05	0.13	0.53	0.15
14400	0.27	0.07	1.00	0.17	0.29	0.62	0.64	0.02	0.08	0.32	0.09
21600	0.25	0.06	0.82	0.17	0.28	0.53	0.64	0.02	0.06	0.18	0.08
28800	0.26	0.06	0.70	0.17	0.26	0.44	0.64	0.02	0.05	0.11	0.08
36000	0.27	0.06	0.62	0.17	0.25	0.39	0.64	0.02	0.04	0.07	0.07
43200	0.29	0.06	0.53	0.17	0.23	0.32	0.64	0.02	0.03	0.04	0.07
54000	0.32	0.06	0.47	0.17	0.23	0.27	0.64	0.02	0.03	0.02	0.07
72000	0.35	0.06	0.38	0.16	0.22	0.21	0.62	0.02	0.02	0.01	0.06

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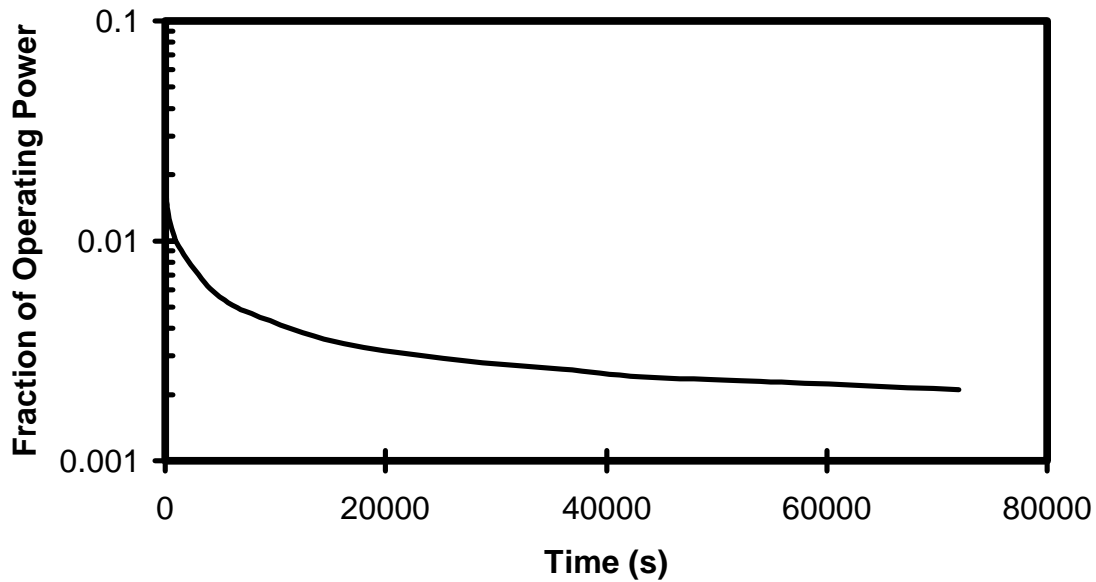


Figure 8.1. Total decay power after reactor shutdown.

8.3 Condensed- and Gas-Phase Data

Table 8.3 contains an alphabetized listing of all of the species in the VICTORIA database. This table contains the common symbol, information about the condensed-phase species, and information about the gas-phase species in the database. Condensed-phase species have the letter “c” as a suffix; gas-phase species have the letter “g” as a suffix. Each species has two numbers attached to it. The first of these is a number in a common set of species that includes all phases; the second is a number in the set of condensed- or gas-phase species, whichever is relevant. Other information in this table is the phase assignment for the condensed-phase species and the set of hydroxide vapors that are normally eliminated from the set of vapor-phase species. The three condensed phases indicated are active only when three condensed phases are being modeled, as described in Section 6.2. Each of the hydroxide vapors indicated by “x” in the column labeled “Elim.” is not treated unless the NAMELIST parameter, `jacksn`, is set to zero (0), as described in Subsection 6.3.8.

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Table 8.3: Species Names and Numbers in VICTORIA Database

Common Symbol	Condensed-Phase Species				Vapor-Phase Species			
	Name	Sp. No.	C-Sp. No.	Phase	Name	Sp. No.	G-Sp. No.	Elim.
Ag	Agc	100	47	1	Agg	99	53	
AgI	AgIc	242	104	3	AgIlg	243	139	
AgOH					AgOHg	244	140	x
Ag(OH) ₂					AgH2O2g	245	141	x
AgTe					AgTeg	101	54	
Ag ₂ Te	Ag2Tec	102	48	1				
Ar					Arg	288	178	
B	Bc	103	49	1	Bg	104	55	
B ₂					B2g	246	142	
BH					BHg	248	144	
BH ₂					BH2g	249	145	
BH ₃					BH3g	250	146	
B ₂ H ₆					B2H6g	251	147	
BI					BIg	105	56	
BI ₂					BI2g	106	57	
BI ₃					BI3g	107	58	
BO					BOg	108	59	
BO ₂					BO2g	109	60	
B ₂ O ₃	B2O3c	110	50	2	B2O3g	111	61	
BOH					BOHg	247	143	x
B(OH) ₂					BH2O2g	252	148	x
BTe					BTeg	112	62	
Ba	Bac	22	11	1	Bag	21	11	
Ba ₂					Ba2g	194	101	
BaH					BaHg	191	99	

Thermochemical and Physical Data

Table 8.3: Species Names and Numbers in VICTORIA Database

Common Symbol	Condensed-Phase Species				Vapor-Phase Species			
	Name	Sp. No.	C-Sp. No.	Phase	Name	Sp. No.	G-Sp. No.	Elim.
BaH ₂	BaH2c	193	93	1				
BaI					BaI _g	18	9	
BaI ₂	BaI2c	20	10	3	BaI2 _g	19	10	
BaMoO ₄	BaMoO4c	26	15	2	BaMoO4 _g	196	103	
BaO	BaOc	17	9	2	BaO _g	16	8	
Ba ₂ O					Ba2O _g	192	100	
Ba ₂ O ₂					Ba2O2 _g	195	102	
BaOH					BaOH _g	13	6	
Ba(OH) ₂	BaO2H2c	15	8	2	BaO2H2 _g	14	7	
BaTe	BaTec	23	12	1				
BaUO ₄	BaUO4c	25	14	2				
BaZrO ₃	BaZrO3c	24	13	2				
Cd	Cdc	120	55	1	Cd _g	119	65	
CdI					CdI _g	255	151	
CdI ₂	CdI2c	256	105	3	CdI2 _g	257	152	
CdO	CdOc	121	56	2	CdO _g	122	66	
CdOH					CdOH _g	253	149	x
Cd(OH) ₂					CdH2O2 _g	254	150	x
CdTe	CdTec	123	57	1	CdTeg	124	67	
Cr	Crc	126	58	1	Cr _g	125	68	
CrI					CrI _g	263	158	
CrI ₂	CrI2c	264	106	3	CrI2 _g	265	159	
CrO					CrO _g	260	155	
CrO ₂					CrO2 _g	261	156	
CrO ₃					CrO3 _g	262	157	
Cr ₂ O ₃	Cr2O3c	127	59	2				

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Table 8.3: Species Names and Numbers in VICTORIA Database

Common Symbol	Condensed-Phase Species				Vapor-Phase Species			
	Name	Sp. No.	C-Sp. No.	Phase	Name	Sp. No.	G-Sp. No.	Elim.
CrOH					CrOHg	258	153	x
Cr(OH) ₂					CrH2O2g	259	154	x
CrTe	CrTec	128	60	1				
Cs	Csc	8	3	1	Csg	5	3	
Cs ₂					Cs2g	167	89	
CsBO ₂	CsBO2c	113	51	2	CsBO2g	169	91	
Cs ₂ CrO ₄	Cs2CrO4c	185	90	2	Cs2CrO4g	182	94	
Cs ₂ Cr ₂ O ₇	Cs2Cr2O7c	184	89	2				
Cs ₃ CrO ₄	Cs3CrO4c	186	91	2				
Cs ₄ CrO ₄	Cs4CrO4c	187	92	2				
CsH					CsHg	168	90	
CsI	Cslc	1	1	3	Cslg	2	1	
Cs ₂ I ₂					Cs2I2g	181	93	
Cs ₂ MoO ₄	Cs2MoO4c	12	7	2	Cs2MoO4g	183	95	
CsO					CsOg	166	88	
Cs ₂ O	Cs2Oc	9	4	2	Cs2Og	6	4	
Cs ₂ O ₂					Cs2O2g	180	92	
CsOH	CsOHc	3	2	2	CsOHg	4	2	
Cs ₂ (OH) ₂					Cs2O2H2g	7	5	
Cs ₂ Te	Cs2Tec	174	83	1				
Cs ₂ TeO ₃	Cs2TeO3c	175	84	2				
Cs ₂ TeO ₄	Cs2TeO4c	178	87	2				
Cs ₂ Te ₂ O ₅	Cs2Te2O5c	176	85	2				
Cs ₂ Te ₄ O ₉	Cs2Te4O9c	177	86	2				
Cs ₂ Te ₄ O ₁₂	Cs2Te4O12c	179	88	2				
Cs ₂ UO ₄	Cs2UO4c	10	5	2				

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Table 8.3: Species Names and Numbers in VICTORIA Database

Common Symbol	Condensed-Phase Species				Vapor-Phase Species			
	Name	Sp. No.	C-Sp. No.	Phase	Name	Sp. No.	G-Sp. No.	Elim.
Cs ₂ U ₂ O ₇	Cs2U2O7c	11	6	2				
Cs ₂ U ₄ O ₁₂	Cs2U4O12c	170	79	2				
Cs ₂ ZrO ₃	Cs2ZrO3c	171	80	2				
Cs ₂ Zr ₂ O ₅	Cs2Zr2O5c	172	81	2				
Cs ₂ Zr ₃ O ₇	Cs2Zr3O7c	173	82	2				
Eu	Euc	157	76	1	Eug	156	81	
EuO	EuOc	159	77	2	EuOg	158	82	
Eu ₂ O					Eu2Og	286	176	
Eu ₂ O ₂					Eu2O2g	287	177	
Eu ₂ O ₃	Eu2O3c	160	78	2				
EuOH					EuOHg	284	174	x
Eu(OH) ₂					EuH2O2g	285	175	x
EuTe					EuTeg	161	83	
Fe	Fec	81	37	1	Feg	82	45	
FeI ₂	FeI2c	87	41	3	FeI2g	88	47	
Fe ₂ I ₄					Fe2I4g	89	48	
FeO	FeOc	83	38	2	FeOg	84	46	
Fe ₂ O ₃	Fe2O3c	85	39	2				
Fe ₃ O ₄	Fe3O4c	86	40	2				
FeOH					FeOHg	223	124	
Fe(OH) ₂	FeO2H2c	225	100	2	FeO2H2g	224	125	
FeTe	FeTec	90	42	1				
FeTe ₂	FeTe2c	91	43	1				
H					Hg	30	15	
H ₂					H2g	31	16	
HBO ₂	HBO2c	114	52	2	HBO2g	115	63	

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Table 8.3: Species Names and Numbers in VICTORIA Database

Common Symbol	Condensed-Phase Species				Vapor-Phase Species			
	Name	Sp. No.	C-Sp. No.	Phase	Name	Sp. No.	G-Sp. No.	Elim.
H ₃ BO ₃	H3BO3c	116	53	2	H3BO3g	117	64	
HI					HIg	29	14	
HIO					HIOg	190	98	
H ₂ MoO ₄					H2MoO4g	164	86	
HO					HOg	189	97	
H ₂ O					H2Og	32	17	
H ₂ Te					H2Teg	69	38	
H ₂ TeO ₃					TeO3H2g	211	115	
H ₂ TeO ₄	TeH2O4c	215	98	2				
He					Heg	165	87	
I					Ig	27	12	
I ₂					I2g	28	13	
IO					IOg	188	96	
In	Inc	130	61	1	Ing	129	69	
InI	InIc	266	107	3	InIg	267	160	
In ₂ O					In2Og	233	130	
In ₂ O ₃	In2O3c	131	62	2				
InOH					InOHg	134	71	x
In(OH) ₂					InH2O2g	268	161	x
InTe	InTec	132	63	1	InTeg	133	70	
Kr					Krg	77	41	
Mn	Mnc	136	64	1	Mng	135	72	
MnO	MnOc	137	65	2	MnOg	269	162	
Mn ₃ O ₄	Mn3O4c	138	66					
MnOH					MnOHg	270	163	x
MnTe	MnTec	139	67	1				

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Table 8.3: Species Names and Numbers in VICTORIA Database

Common Symbol	Condensed-Phase Species				Vapor-Phase Species			
	Name	Sp. No.	C-Sp. No.	Phase	Name	Sp. No.	G-Sp. No.	Elim.
MnTe ₂	MnTe2c	140	68	1				
Mo	Moc	92	44	1	Mog	93	49	
Mo ₂					Mo2g	229	126	
MoI					Molg	234	131	
MoI ₂	MoI2c	228	103	3	MoI2g	235	132	
MoI ₃	MoI3c	227	102	3	MoI3g	236	133	
MoI ₄	MoI4c	226	101		MoI4g	241	138	
MoO					MoOg	94	50	
MoO ₂	MoO2c	95	45	2	MoO2g	96	51	
MoO ₃	MoO3c	97	46	2	MoO3g	98	52	
Mo ₂ O ₆					Mo2O6g	230	127	
Mo ₃ O ₉					Mo3O9g	238	135	
Mo ₄ O ₁₂					Mo4O12g	239	136	
Mo ₅ O ₁₅					Mo5O15g	240	137	
MoOH					MoOHg	231	128	x
Mo(OH) ₂					MoH2O2g	232	129	x
MoO ₂ I ₂					MoO2I2g	237	134	
Ni	Nic	142	69	1	Nig	141	73	
Nil ₂	Nil2c	274	108	3				
NiO	NiOc	143	70	2	NiOg	271	164	
NiOH					NiOHg	272	165	x
Ni(OH) ₂					NiH2O2g	273	166	x
O					Og	80	44	
O ₂					O2g	79	43	
Ru	Ruc	145	71	1	Rug	144	74	
RuO					RuOg	278	168	

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Table 8.3: Species Names and Numbers in VICTORIA Database

Common Symbol	Condensed-Phase Species				Vapor-Phase Species			
	Name	Sp. No.	C-Sp. No.	Phase	Name	Sp. No.	G-Sp. No.	Elim.
RuO ₂	RuO2c	146	72	2	RuO2g	277	167	
RuO ₃					RuO3g	147	75	
RuO ₄					RuO4g	148	76	
RuOH					RuOHg	279	169	x
Ru(OH) ₂					RuH2O2g	280	170	x
RuTe ₂	RuTe2c	276	110	1				
Ru ₃ U	Ru3Uc	275	109	1				
Sb	Sbc	150	73	1	Sbg	149	77	
Sb ₂					Sb2g	151	78	
Sb ₄					Sb4g	152	78	
SbH ₃					SbH3g	283	173	
Sb ₂ O ₃	Sb2O3c	153	74	2				
SbOH					SbOHg	281	171	x
Sb(OH) ₂					SbH2O2g	282	172	x
SbTe					SbTeg	154	80	
Sb ₂ Te ₃	Sb2Te3c	155	75	1				
Sn	Snc	51	25	1	Sng	52	27	
Sn ₂					Sn2g	209	113	
SnH ₄					SnH4g	61	32	
SnI ₂	SnI2c	58	28	3	SnI2g	57	30	
SnO	SnOc	54	26	2	SnOg	53	28	
SnO ₂	SnO2c	55	27	2	SnO2g	56	29	
SnOH					SnOHg	207	111	x
Sn(OH) ₂					SnH2O2g	208	112	x
SnTe	SnTec	60	29	1	SnTeg	59	31	
SnTe ₂					SnTe2g	210	114	

Thermochemical and Physical Data

Table 8.3: Species Names and Numbers in VICTORIA Database

Common Symbol	Condensed-Phase Species				Vapor-Phase Species			
	Name	Sp. No.	C-Sp. No.	Phase	Name	Sp. No.	G-Sp. No.	Elim.
Sn ₂ Te ₂					Sn2Te2g	163	85	
Sr	Src	42	19	1	Srg	41	23	
Sr ₂					Sr2g	198	104	
SrH ₂	SrH2c	197	94	1				
Srl					Srlg	38	21	
Srl ₂	Srl2c	40	18	3	Srl2g	39	22	
SrMoO ₄	SrMoO4c	45	22	2				
SrO	SrOc	36	17	2	SrOg	37	20	
SrOH					SrOHg	33	18	
Sr(OH) ₂	SrO2H2c	34	16	2	SrO2H2g	35	19	
SrUO ₄	SrUO4c	43	20	2				
SrZrO ₃	SrZrO3c	44	21	2				
Te	Tec	63	30	1	Teg	62	33	
Te ₂					Te2g	64	34	
Tel ₄	Tel4c	214	97	3	Tel4g	212	116	
TeO					TeOg	65	35	
TeO ₂	TeO2c	67	31	2	TeO2g	66	36	
Te ₂ O ₂					Te2O2g	68	37	
TeOH					TeOHg	216	118	x
Te(OH) ₂					TeH2O2g	217	119	x
TeOI ₂					TeOI2g	213	117	
U	Uc	72	33	1	Ug	73	40	
UO					UOg	219	120	
UO ₂	UO2c	70	32	2	UO2g	71	39	
UO ₃	UO3c	76	36	2	UO3g	220	121	
U ₃ O ₈	U3O8c	75	35	2				

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Table 8.3: Species Names and Numbers in VICTORIA Database

Common Symbol	Condensed-Phase Species				Vapor-Phase Species			
	Name	Sp. No.	C-Sp. No.	Phase	Name	Sp. No.	G-Sp. No.	Elim.
U ₄ O ₉	U4O9c	74	34	2				
UOH					UOHg	221	122	x
U(OH) ₂					UH2O2g	222	123	x
UO ₃ ·2H ₂ O	UH4O5c	218	99	2				
Xe					Xeg	78	42	
Zr	Zrc	50	24	1	Zrg	49	26	
ZrB ₂	ZrB2c	118	54	1				
ZrH					ZrHg	162	84	
ZrI					Zrlg	204	108	
ZrI ₂					Zrl2g	203	107	
ZrI ₃					Zrl3g	202	106	
ZrI ₄	Zrl4c	199	95	3	Zrl4g	201	105	
ZrO					ZrOg	46	24	
ZrO ₂	ZrO2c	48	23	2	ZrO2g	47	25	
ZrOH					ZrOHg	205	109	x
Zr(OH) ₂					ZrH2O2g	206	110	x
ZrTe ₂	ZrTe2c	200	96	1				

8.4 Gibbs Free Energy Data

Table 8.4 shows the Gibbs free energy data in the VICTORIA database. References for each species are given in the footnotes. Gibbs free energy in units of kcal/g-mol are calculated from the following polynomial, with temperature, T , measured in degrees kelvin:

$$G = a + bT + cT^2 + dT^3 \quad (8.1)$$

Gibbs free energies are converted within the code to J/kg-mol by multiplying by $4.184 \cdot 10^6$.

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Table 8.4: Gibbs Free Energy Data in the VICTORIA Database

Species Name	Gibbs Free Energy Coefficients				Species Name	Gibbs Free Energy Coefficients			
	a	b·10 ³	c·10 ⁶	d·10 ⁹		a	b·10 ³	c·10 ⁶	d·10 ⁹
Cslc ^a	-73.64	-35.89	-8.181	-0.1583	Ruc ^a	2.48	-10.56	-1.710	-0.1676
Cslg ^a	-25.24	-74.01	-4.486	0.3432	RuO2c ^a	-67.79	-18.92	-9.222	0.6071
CsOHc ^b	-90.10	-36.35	-9.405	0.7195	RuO3g ^a	-13.02	-71.51	-9.267	0.6827
CsOHg ^b	-57.92	-65.17	-6.490	0.4750	RuO4g ^a	-36.71	-76.49	-11.960	0.8828
Csg ^b	20.32	-44.07	-2.334	0.1679	Sbg ^a	64.99	-45.14	-2.344	0.1643
Cs2Og ^b	-37.46	-74.35	-10.690	1.1890	Sbc ^a	6.85	-18.07	-3.621	0.2773
Cs2O2H2g ^b	-157.90	-91.41	-13.420	0.9649	Sb2g ^a	55.12	-59.01	-4.705	0.7373
Csc ^b	3.13	-25.06	-3.567	0.2729	Sb4g ^a	49.21	-81.56	-5.228	0.8191
Cs2Oc ^b	-79.28	-44.96	0.000	0.0000	Sb2O3c ^a	-146.60	-55.53	-18.100	1.3870
Cs2UO4c ^c	-440.50	-65.80	-20.950	1.4440	SbTeg ^h	48.10	-59.18	-9.215	1.4230
Cs2U2O7c ^d	-713.40	-141.10	-37.600	2.5890	Sb2Te3c ^h	-16.99	-32.76	-50.060	11.3600
Cs2MoO4c ^e	-350.60	-68.15	-24.690	1.3490	Eug ^a	43.86	-47.46	-2.225	0.1509
BaOHg ^b	-50.14	-64.50	-6.352	0.4498	Euc ^a	3.97	-21.71	-4.593	0.3635
BaO2H2g ^a	-143.30	-81.61	-11.010	0.7971	EuOg ^a	-7.33	-64.42	-4.345	0.3328
BaO2H2c ^a	-213.20	-35.67	-16.250	1.2440	EuOc ^a	-130.40	-24.25	-6.262	0.4306
BaOg ^b	-26.45	-59.81	-4.047	0.2781	Eu2O3c ^a	-402.20	-44.68	-17.640	1.2830
BaOc ^a	-135.30	-10.93	-10.160	0.6290	EuTeg ^h	34.62	-65.71	-9.422	1.4770
Balg ^b	-3.86	-65.37	-6.955	0.7395	ZrHg ⁱ	124.00	-51.05	-5.608	0.5140
Bal2g ^b	-66.90	-84.85	-10.830	1.2110	Sn2Te2g ⁱ	42.74	-94.41	-13.650	1.3330
Bal2c ^a	-131.70	-51.18	-13.020	0.9963	H2MoO4g ⁱ	-201.50	-81.67	-22.110	2.0130
Bag ^a	45.81	-44.00	-1.430	-0.0611	Heg	0.00	0.00	0.000	0.0000
Bac ^a	5.15	-20.15	-4.679	0.3580	CsOg ^j	-13.00	-12.63	-34.362	5.6966
BaTec ^a	-60.86	-27.42	-5.920	0.3764	Cs2g ^k	25.45	-65.76	-7.702	0.8378
BaZrO3c ^a	-414.10	-35.46	-15.070	1.0680	CsHg ^j	27.61	-49.04	-7.160	0.7788
BaUO4c ^f	-465.40	-49.43	-18.820	1.0720	CsBO2g ^k	-166.85	-71.46	-14.422	1.5443

Thermochemical and Physical Data

Table 8.4: Gibbs Free Energy Data in the VICTORIA Database

Species Name	Gibbs Free Energy Coefficients				Species Name	Gibbs Free Energy Coefficients			
	a	b·10 ³	c·10 ⁶	d·10 ⁹		a	b·10 ³	c·10 ⁶	d·10 ⁹
BaMoO ₄ c ^a	-350.60	-42.79	-18.620	1.1540	Cs ₂ U ₄ O ₁₂ ^k	-1341.20	-57.98	-133.740	22.6560
Ig ^a	27.27	-45.20	-2.401	0.1800	Cs ₂ ZrO ₃ c ^k	-419.76	-26.76	-48.113	6.6312
I ₂ g ^a	18.06	-65.86	-4.376	0.3295	Cs ₂ Zr ₂ O ₅ ^k	-684.30	-32.87	-69.522	10.0110
HIg ^a	8.53	-51.63	-3.749	0.2327	Cs ₂ Zr ₃ O ₇ ^k	-946.34	-37.24	-90.932	13.3910
Hg ^a	53.87	-29.44	-2.396	0.1833	Cs ₂ Te ^j	-103.15	-5.63	-36.605	5.1790
H ₂ g ^a	2.31	-33.73	-3.538	0.2409	Cs ₂ TeO ₃ c ^j	-258.47	-3.12	-55.596	6.9026
H ₂ Og ^a	-55.34	-47.34	-4.740	0.2648	Cs ₂ Te ₂ O ₅ ^j	-350.90	-2.81	-77.632	10.1700
SrOHg ^b	-45.21	-62.84	-6.408	0.4624	Cs ₂ Te ₄ O ₉ ^j	-526.73	0.03	-121.730	14.1350
SrO ₂ H ₂ c ^b	-219.00	-32.31	-18.180	1.3910	Cs ₂ TeO ₄ c ^j	-288.81	-0.45	-61.186	6.7928
SrO ₂ H ₂ g ^b	-136.00	-79.10	-11.000	0.7962	Cs ₂ Te ₄ O ₁ ^j	-600.33	2.95	-129.900	16.8210
SrOc ^a	-144.70	-7.40	-13.001	1.9033	Cs ₂ O ₂ g ^j	33.87	-12.69	-47.335	7.4792
SrOg ^a	-0.29	-58.46	-3.792	0.1433	Cs ₂ I ₂ g ^j	-149.39	-21.14	-62.332	10.1730
SrI ₂ g ^b	-4.11	-68.64	-4.403	0.3275	Cs ₂ CrO ₄ g ⁱ	-305.63	-15.66	-73.187	11.2210
SrI ₂ g ^b	-60.45	-87.18	-7.183	0.5493	Cs ₂ MoO ₄ g ⁱ	-326.36	-15.77	-73.607	11.2940
SrI ₂ c ^a	-123.10	-49.30	-13.020	0.9963	Cs ₂ Cr ₂ O ₇ ^j	-535.26	19.90	-118.320	16.3660
Srg ^a	41.94	-41.73	-2.399	0.1835	Cs ₂ CrO ₄ c ^j	-366.66	10.60	-70.739	9.7008
Src ^a	4.95	-17.57	-3.613	0.2791	Cs ₃ CrO ₄ c ^j	-398.10	1.17	-77.550	10.0740
SrUO ₄ c ^g	-469.20	-46.02	-18.640	1.0500	Cs ₄ CrO ₄ c ^j	-412.46	-9.00	-81.529	9.2757
SrZrO ₃ c ^a	-416.00	-34.60	-15.310	1.0540	IOg ^k	42.54	-54.59	-7.635	0.8340
SrMoO ₄ c ^a	-360.50	-39.30	-18.830	1.1670	HOg ^k	9.36	-42.17	-5.907	0.6237
ZrOg ^a	14.32	-52.97	-6.391	0.5210	HIog ^j	-41.65	-12.40	-35.983	5.8127
ZrO ₂ g ^b	-95.06	-60.39	-10.010	1.0780	BaHg ^k	53.01	-50.05	-6.818	0.7160
ZrO ₂ c ^a	-246.70	-33.11	-0.774	-0.6911	Ba ₂ Og ^k	-57.66	-65.31	-11.877	1.3203
Zrg ^a	150.50	-45.98	-2.989	0.1971	BaH ₂ c ^j	-43.75	-5.62	-15.569	3.2025
Zrc ^a	0.19	-7.95	-5.370	0.3999	Ba ₂ g ^j	57.19	-16.48	-35.597	6.1375
Snc ^a	4.12	-18.40	-3.280	0.2509	Ba ₂ O ₂ g ^j	-100.33	-14.23	-49.706	7.9087

Thermochemical and Physical Data

Table 8.4: Gibbs Free Energy Data in the VICTORIA Database

Species Name	Gibbs Free Energy Coefficients				Species Name	Gibbs Free Energy Coefficients			
	a	b·10 ³	c·10 ⁶	d·10 ⁹		a	b·10 ³	c·10 ⁶	d·10 ⁹
Sng ^a	75.91	-43.91	-3.045	0.2330	BaMoO4g ^j	-264.84	-14.28	-63.340	9.7585
SnOg ^a	7.78	-58.43	-4.200	0.3083	SrH2c ^j	-44.08	-3.97	-15.430	3.1850
SnOc ^a	-65.06	-16.40	-6.356	0.3524	Sr2g ^j	49.34	-15.71	-34.338	5.9104
SnO2c ^a	-133.10	-17.61	-9.586	0.6367	ZrI4c ^j	-139.47	-6.81	-53.089	7.6658
SnO2g ^a	-9.97	-57.37	-10.990	1.2000	ZrTe2c ^j	-81.48	-2.56	-28.918	4.0010
SnI2g ^a	3.68	-85.48	-7.099	0.5350	ZrI4g ^j	-124.95	-20.53	-68.830	11.0320
SnI2c ^a	-3.55	-71.53	-10.900	0.8339	ZrI3g ^j	-66.85	-19.28	-58.995	9.5742
SnTeg ^a	40.34	-65.95	-4.318	0.3305	ZrI2g ^j	1.36	-17.27	-49.165	8.0650
SnTec ^a	-1.18	-35.31	-8.172	0.6757	ZrIg ^j	71.00	-14.53	-36.717	6.1374
SnH4g ^a	42.29	-55.78	-10.400	0.4490	ZrOHg ^j	7.45	-12.80	-36.305	5.8773
Teg ^a	52.27	-45.51	-2.463	0.1717	ZrH2O2g ^j	-124.38	-12.55	-45.295	6.9720
Tec ^a	6.65	-19.65	-4.341	0.3321	SnOHg ^j	-21.72	-12.68	-36.332	5.8788
Te2g ^a	40.89	-65.19	-4.788	0.3054	SnH2O2g ^j	-119.63	-11.60	-45.049	6.9069
TeOg ^a	20.60	-60.49	-4.210	0.3090	Sn2g ^j	75.75	-12.50	-37.161	6.1089
TeO2g ^a	-12.78	-62.62	-10.150	1.0980	SnTe2g ^j	67.32	-15.65	-46.316	7.5529
TeO2c ^a	-67.75	-23.24	-13.250	0.9942	TeO3H2g ^j	-132.47	-13.07	-55.850	8.5324
Te2O2g ^a	-19.72	-84.55	-10.060	0.7160	Tel4g ^j	-27.06	-21.13	-69.948	11.2330
H2Teg ^a	26.52	-56.99	-5.511	0.3108	TeOI2g ^j	-42.81	-17.60	-55.584	8.9661
UO2c ^a	-253.40	-24.14	-9.969	0.6970	Tel4c ^j	-34.17	-7.63	-56.584	8.4285
UO2g ^a	-109.20	-64.62	-9.969	0.6970	TeH2O4c ^j	-180.24	8.52	-42.722	1.9093
Uc ^a	2.85	-12.51	-6.735	0.5827	TeOHg ^j	-32.37	-13.05	-37.436	6.0713
Ug ^a	119.40	-42.64	-5.099	0.3901	TeH2O2g ^j	-100.03	-12.00	-44.931	6.8977
U4O9c ^a	-1052.00	-105.30	-44.900	3.0960	UH4O5c ^j	-453.83	9.40	-69.133	5.0499
U3O8c ^a	-833.50	-86.98	-36.670	2.4560	UOg ^j	-11.77	-11.42	-35.194	5.6250
UO3c ^a	-286.90	-30.53	-11.850	0.8065	UO3g ^j	-204.04	-13.72	-50.159	7.7265
Krg	0.00	0.00	0.000	0.0000	UOHg ^j	-1.89	-13.15	-39.067	6.3105

Thermochemical and Physical Data

Table 8.4: Gibbs Free Energy Data in the VICTORIA Database

Species Name	Gibbs Free Energy Coefficients				Species Name	Gibbs Free Energy Coefficients			
	a	b·10 ³	c·10 ⁶	d·10 ⁹		a	b·10 ³	c·10 ⁶	d·10 ⁹
Xeg	0.00	0.00	0.000	0.0000	UH2O2g ^j	-108.65	-13.76	-48.396	7.5152
O2g ^a	2.41	-51.47	-3.943	0.2630	FeOHg ^j	-16.22	-65.27	-14.051	2.1352
Og ^a	61.38	-40.64	-2.404	0.1839	FeO2H2g ^j	-104.26	-10.92	-47.949	7.3230
Fec ^a	-0.61	-2.83	-7.397	0.6513	FeO2H2c ^j	-145.23	2.28	-31.977	4.1446
Feg ^a	99.52	-44.11	-3.120	0.2387	MoI4c ^j	-65.95	-7.80	-56.012	8.3606
FeOc ^a	-67.30	-7.12	-12.860	1.2350	MoI3c ^j	-60.09	-4.63	-43.548	6.1780
FeOg ^b	62.79	-60.72	-4.223	0.3089	MoI2c ^j	-39.79	-3.63	-33.281	4.7304
Fe2O3c ^a	-185.00	-33.55	-16.170	1.1700	Mo2g ^j	196.59	-12.53	-33.156	5.4919
Fe3O4c ^a	-283.60	1.78	-49.170	4.7480	Mo2O6g ^j	-303.97	-13.45	-75.784	11.3910
FeI2c ^a	-7.38	-57.84	-13.020	0.9963	MoOHg ^j	48.40	-13.01	-36.429	5.9032
FeI2g ^a	26.06	-89.19	-7.293	0.5282	MoH2O2g ^j	-68.75	-11.70	-43.048	6.5804
Fe2I4g ^a	13.04	-142.50	-15.450	1.1470	In2Og ^j	-235.00	-12.59	-63.525	9.5666
FeTec ^a	-1.32	-23.60	-6.575	0.4634	MoIg ^j	94.70	-14.68	-36.953	6.1623
FeTe2c ^a	-11.60	-29.13	-10.770	0.6349	MoI2g ^j	31.93	-16.53	-49.962	8.1739
Moc ^a	4.80	-13.86	-0.400	-0.3243	MoI3g ^j	7.79	-19.38	-59.359	9.5949
Mog ^a	159.50	-45.94	-2.136	0.1312	MoO2I2g ^j	-145.49	-15.48	-58.825	9.2462
MoOg ^a	85.68	-57.15	-6.815	0.7462	Mo3O9g ^j	-493.57	-16.13	-109.290	16.1940
MoO2c ^a	-136.40	-14.85	-9.593	0.4909	Mo4O12g ^j	-672.78	-17.42	-140.460	20.5800
MoO2g ^a	0.26	-68.84	-6.486	0.3099	Mo5O15g ^j	-847.33	-18.42	-171.150	24.8730
MoO3c ^a	-162.70	-29.64	-15.250	1.2040	MoI4g ^j	-10.49	-20.93	-69.501	11.1520
MoO3g ^a	-80.75	-72.03	-9.368	0.7082	AgIc ^k	-10.67	-30.67	-11.714	1.3494
Agg ^h	69.68	-43.37	-2.398	0.1837	AgIg ^k	33.07	-60.96	-7.504	0.8430
Agc ^h	2.47	-11.14	-4.923	0.4390	AgOHg ^j	-13.42	-10.71	-34.481	5.4895
AgTeg ^a	71.80	-63.33	-7.133	0.7673	AgH2O2g ^j	-38.92	-12.09	-43.737	6.7041
Ag2Tec ^a	-3.34	-51.55	0.000	0.0000	B2g ^j	181.59	-9.64	-29.004	4.6831
Bc ^a	1.00	-2.19	-2.341	-0.0143	BOHg ^j	-19.87	-8.78	-30.243	4.7390

Thermochemical and Physical Data

Table 8.4: Gibbs Free Energy Data in the VICTORIA Database

Species Name	Gibbs Free Energy Coefficients				Species Name	Gibbs Free Energy Coefficients			
	a	b·10 ³	c·10 ⁶	d·10 ⁹		a	b·10 ³	c·10 ⁶	d·10 ⁹
Bg ^a	135.30	-35.97	-3.875	0.4337	BHg ^k	105.76	-39.02	-6.213	0.6492
Blg ⁱ	73.78	-55.40	-5.937	0.5618	BH2g ^k	47.75	-39.50	-8.888	0.8769
Bl2g ⁱ	59.11	-73.46	-9.052	0.8595	BH3g ^k	-25.90	-40.58	-9.798	0.8704
Bl3g ⁱ	18.62	-82.66	-12.960	1.2320	B2H6g ^j	8.34	-44.24	-22.212	1.9594
BOg ⁱ	0.52	-48.09	-5.294	0.4781	BH2O2g ^j	-133.39	-10.48	-38.513	5.8035
BO2g ⁱ	-67.20	-53.55	-9.145	0.8452	CdOHg ^j	-30.46	-11.29	-35.837	5.7296
B2O3c ⁱ	-295.20	-18.96	-17.470	1.5580	CdH2O2g ^j	-114.02	-11.32	-42.640	6.5034
B2O3g ⁱ	-198.10	-64.99	-14.930	1.3440	Cdlg ^k	36.82	-62.98	-7.559	0.8431
BTeg ^h	98.66	-53.00	-8.882	1.3510	CdI2c ^k	-44.73	-37.39	-20.049	2.2532
CsBO2c ⁱ	-227.40	-20.30	-23.850	2.6840	CdI2g ^k	-13.37	-74.87	-12.341	1.3880
HBO2c ⁱ	-193.20	-1.36	-19.900	2.9240	CrOHg ^j	1.64	-12.49	-35.525	5.7406
HBO2g ⁱ	-133.50	-54.68	-10.220	0.8761	CrH2O2g ^j	-94.71	-10.62	-41.271	6.2586
H3BO3c ⁱ	-264.00	-3.23	-33.440	4.5840	CrOg ^j	23.72	-12.24	-32.292	5.3391
H3BO3g ⁱ	-237.20	-58.19	-19.370	1.6730	CrO2g ^j	-41.97	-12.83	-38.825	6.2724
ZrB2c ⁱ	-76.90	-4.84	-12.520	1.2500	CrO3g ^k	-93.74	-11.08	-42.660	6.6595
Cdg ^a	27.97	-41.61	-2.398	0.1837	CrIlg ^k	58.06	-62.30	-7.390	0.8229
Cdc ^a	3.86	-17.43	-3.428	0.2625	CrI2c ^k	-30.07	-39.07	-19.569	2.0430
CdOc ^a	-58.24	-16.83	-6.299	0.4229	CrI2g ^k	24.07	-81.26	-12.662	1.4460
CdOg ^a	19.05	-51.82	-9.370	1.4340	InIc ⁱ	-40.31	-0.35	-32.435	5.0585
CdTec ^h	-25.55	-12.25	-20.320	4.4100	InIg ⁱ	1.60	-60.21	-9.495	1.4725
CdTeg ^h	57.79	-60.03	-9.313	1.4490	InH2O2g ^j	-129.84	-12.43	-46.769	7.2132
Crg ^a	96.79	-43.85	-2.191	0.1135	MnOg ^k	30.97	-54.38	-7.096	0.7842
Crc ^a	-2.21	-0.68	-6.681	0.5393	MnOHg ^j	-18.83	-12.61	-35.733	5.7780
Cr2O3c ^a	-252.90	-44.70	-4.475	-1.0610	NiOg ^j	54.94	-11.41	-30.837	5.0746
CrTec ^h	-20.76	-26.67	0.000	0.0000	NiOHg ^j	12.40	-11.45	-35.745	5.7172
Ing ^a	60.52	-43.92	-2.795	0.2140	NiH2O2g ^j	-86.28	-11.80	-44.207	6.7720

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Table 8.4: Gibbs Free Energy Data in the VICTORIA Database

Species Name	Gibbs Free Energy Coefficients				Species Name	Gibbs Free Energy Coefficients			
	a	b·10 ³	c·10 ⁶	d·10 ⁹		a	b·10 ³	c·10 ⁶	d·10 ⁹
Inc ^a	3.23	-18.43	-3.355	0.2570	Nil2c ^k	-11.42	-31.78	-19.779	2.0795
In2O3c ^a	-222.80	-19.54	-20.750	1.4000	Ru3Uc ^j	-49.67	-1.60	-37.560	5.0972
InTec ^h	-12.06	-37.44	0.000	0.0000	RuTe2c ^j	-42.47	-1.04	-25.504	3.4434
InTeg ^h	57.13	-61.20	-9.430	1.4790	RuO2g ^j	8.69	-12.70	-38.791	6.2639
InOHg ⁱ	-40.52	-11.53	-36.347	5.8202	RuOg ^j	68.33	-12.43	-32.593	5.4009
Mng ^a	69.40	-43.45	-2.418	0.1852	RuOHg ^j	56.16	-13.30	-36.945	5.9960
Mnc ^a	0.32	-4.22	-7.824	0.7346	RuH2O2g ^j	-27.36	-12.26	-44.017	6.7547
MnOc ^a	-98.83	-1.67	-13.390	1.1500	SbOHg ^j	-24.92	-12.31	-35.527	5.7364
Mn3O4c ^a	-348.30	5.74	-49.870	4.9540	SbH2O2g ^j	-109.10	-12.28	-45.051	6.9246
MnTec ^h	-27.66	-13.52	-18.810	3.8540	SbH3g ^j	33.67	-48.13	-15.130	2.2863
MnTe2c ^h	-27.14	-43.37	0.000	0.0000	EuOHg ^j	-191.78	-12.54	-37.800	6.0848
Nig ^a	105.30	-46.47	-2.584	0.1979	EuH2O2g ^j	-194.74	-12.55	-45.163	6.9503
Nic ^a	-2.79	-0.70	-8.139	0.7709	Eu2Og ^j	-65.46	-17.03	-47.011	7.7343
NiOc ^a	-58.49	-6.49	-8.911	0.5167	Eu2O2g ^j	-162.02	-16.85	-53.739	8.6398
Rug ^a	157.20	-46.84	-2.869	0.1945	Arg ^k	0.04	-35.82	-4.151	0.4709

- a. Barin and Kanacke (1977)
- b. Chase et al. (1985)
- c. O'Hare and Hoekstra (1974)
- d. O'Hare et al. (1981)
- e. O'Hare and Hoekstra (1973)
- f. O'Hare et al. (1976)
- g. Tagawa, Fujino, and Yamashita (1979)
- h. Mills (1974)
- i. Ball, Barton, and Mignanelli (1991)
- j. Ball, Mignanelli, and Yates (1992)
- k. Powers (1991)

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8.5 Lennard-Jones Coefficients

Lennard-Jones coefficients are used to calculate gas-phase diffusion coefficients, as described in Subsection 2.1.2. The values that are currently used are taken from Henshaw et al. (1994).

Table 8.5: Lennard-Jones Coefficients for Gas-Phase Species

Species Name	L-J Coeff.		Species Name	L-J Coeff.		Species Name	L-J Coeff.		Species Name	L-J Coeff.	
	σ (Å)	ϵ/κ_B (K)		σ (Å)	ϵ/κ_B (K)		σ (Å)	ϵ/κ_B (K)		σ (Å)	ϵ/κ_B (K)
CsI	4.03	685	FeO	3.68	704	CsBO ₂	4.22	726	Mo ₄ O ₁₂	5.90	379
CsOH	3.90	692	FeI ₂	3.89	1042	Cs ₂ O ₂	6.35	359	Mo ₅ O ₁₅	6.00	377
Cs	4.40	6990	Fe ₂ I ₄	3.82	1050	Cs ₂ I ₂	7.05	279	Mol ₄	5.60	388
Cs ₂ O	3.94	689	Mo	3.65	2770	Cs ₂ CrO ₄	2.53	2644	AgI	3.79	698
Cs(OH) ₂	3.70	854	MoO	3.73	691	Cs ₂ MoO ₄	2.42	2931	AgOH	3.87	693
BaOH	3.89	697	MoO ₂	3.87	747	IO	3.64	813	Ag(OH) ₂	4.81	544
Ba(OH) ₂	5.16	608	MoO ₃	4.33	666	HO	3.59	689	B ₂	3.66	680
BaO	3.84	695	Ag	3.48	1300	HIO	3.86	763	BOH	3.86	711
BaI	3.94	691	AgTe	3.81	431	BaH	3.90	1139	BH	3.65	709
BaI ₂	3.91	777	B	3.13	446	Ba ₂ O	3.92	701	BH ₂	3.86	734
Ba	4.06	18500	BI	3.67	695	Ba ₂	4.15	981	BH ₃	4.44	764
I	3.29	1740	BI ₂	3.88	802	Ba ₂ O ₂	5.75	397	B ₂ H ₆	4.36	633
I ₂	3.74	801	BI ₃	4.92	524	BaMoO ₄	3.94	908	B(OH) ₂	4.60	588
HI	3.69	703	BO	3.60	732	Sr ₂	4.07	933	CdOH	3.87	700
H	3.10	9	BO ₂	3.85	782	ZrI ₄	5.67	376	Cd(OH) ₂	4.80	544
H ₂	3.65	1668	B ₂ O ₃	4.48	648	ZrI ₃	5.49	409	CdI	3.79	709
H ₂ O	3.86	694	BTe	3.72	717	ZrI ₂	3.90	780	CdI ₂	3.89	1008
SrOH	3.88	1305	HBO ₂	4.06	727	ZrI	3.87	700	CrOH	3.87	693
Sr(OH) ₂	5.07	495	H ₃ BO ₃	4.85	542	ZrOH	3.88	699	Cr(OH) ₂	4.83	540
SrO	3.80	697	Cd	3.46	1760	Zr(OH) ₂	4.98	510	CrO	3.70	690
SrI	3.60	731	CdO	3.68	704	SnOH	3.87	721	CrO ₂	3.86	749

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Table 8.5: Lennard-Jones Coefficients for Gas-Phase Species

Species Name	L-J Coeff.		Species Name	L-J Coeff.		Species Name	L-J Coeff.		Species Name	L-J Coeff.	
	σ (Å)	ϵ/κ_B (K)		σ (Å)	ϵ/κ_B (K)		σ (Å)	ϵ/κ_B (K)		σ (Å)	ϵ/κ_B (K)
SrI ₂	3.90	778	CdTe	3.80	697	Sn(OH) ₂	4.81	541	CrO ₃	4.22	702
Sr	3.91	10900	Cr	3.52	2090	Sn ₂	3.84	695	CrI	3.80	697
ZrO	3.76	699	In	3.61	2160	SnTe ₂	3.89	782	CrI ₂	3.89	769
ZrO ₂	3.87	760	InTe	3.84	702	H ₂ TeO ₃	4.10	813	InI	3.83	716
Zr	3.77	6150	InOH	3.87	708	Tel ₄	5.42	426	In(OH) ₂	4.89	525
Sn	3.48	2130	Mn	3.48	2700	TeOI ₂	4.77	569	MnO	3.69	704
SnO	3.69	739	Ni	3.39	1630	TeOH	3.86	748	MnOH	3.87	700
SnO ₂	3.86	792	Ru	3.60	1900	Te(OH) ₂	4.73	562	NiO	3.66	705
SnI ₂	3.89	812	RuO ₃	4.29	680	UO	3.84	695	NiOH	3.87	700
SnTe	3.81	719	RuO ₄	4.62	608	UO ₃	4.71	566	Ni(OH) ₂	4.75	553
SnH ₄	5.06	638	Sb	3.41	1780	UOH	3.89	697	RuO ₂	3.87	748
Te	3.35	1850	Sb ₂	3.81	719	U(OH) ₂	5.17	479	RuO	3.72	691
Te ₂	3.77	756	Sb ₄	5.52	410	FeOH	3.87	700	RuOH	3.87	693
TeO	3.65	787	SbTe	3.79	736	Fe(OH) ₂	4.79	546	Ru(OH) ₂	4.88	531
TeO ₂	3.86	824	Eu	3.99	11800	Mo ₂	3.93	3831	SbOH	3.87	734
Te ₂ O ₂	4.48	650	EuO	3.82	696	Mo ₂ O ₆	4.48	728	Sb(OH) ₂	4.77	551
H ₂ Te	3.87	693	EuTe	3.94	689	MoOH	3.87	693	SbH ₃	4.69	653
UO ₂	3.88	757	ZrH	3.82	1034	Mo(OH) ₂	4.91	526	EuOH	3.89	698
U	4.07	17500	Sn ₂ Te ₂	5.53	409	In ₂ O	4.59	628	Eu(OH) ₂	5.12	487
Kr	3.14	671	H ₂ MoO ₄	4.59	628	Mol	3.84	695	Eu ₂ O	3.91	702
Xe	3.24	1550	He	2.79	4	Mol ₂	3.90	780	Eu ₂ O ₂	5.62	414
O ₂	3.53	820	CsO	3.93	694	Mol ₃	5.39	428	Ar	3.03	359
O	2.89	62	Cs ₂	4.32	11068	MoO ₂ I ₂	5.13	481			
Fe	3.45	2200	CsH	3.99	4474	Mo ₃ O ₉	5.64	412			

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8.6 Species Densities, Melting Points, and Boiling Points

Species densities are used in VICTORIA to calculate the densities of aerosol particles, as described in Subsection 5.2.2. Melting points and boiling points are not at present used in VICTORIA, but are useful for understanding what phase a species would be in at a specified temperature. In particular, it may be useful to know whether aerosols are solid, liquid, or a mixture of both phases. The aerosol resuspension model described in Section 5.7 is intended for applications where the aerosols are entirely in the solid phase.

Data for the elements in Table 8.6 are taken from Emsley (1992); data for the nonelemental species are taken from the *CRC Handbook of Chemistry and Physics, 52nd Ed.* (1971); data that could not be found in either source were assigned a density of 4000 kg/m³, which was chosen to be an average value.

Table 8.6: Density, Melting Point, and Boiling Point for the Condensed-Phase Species

Name	ρ (kg/ m ³)	T _M (K)	T _B (K)	Name	ρ (kg/ m ³)	T _M (K)	T _B (K)	Name	ρ (kg/ m ³)	T _M (K)	T _B (K)
CsI	4510	894	1553	FeO	5700	1693		Sb ₂ Te ₃	6500	902	
CsOH	3675	545		Fe ₂ O ₃	5240	1838		Eu	5243	1095	1870
Cs	1843	952	1843	Fe ₃ O ₄	5180	1811		EuO	4000		
Cs ₂ O	4250	763		FeI ₂	5315			Eu ₂ O ₃	7420		
Cs ₂ UO ₄	4000			FeTe	4000			Cs ₂ U ₄ O ₁₂	4000		
Cs ₂ U ₂ O ₇	4000			FeTe ₂	4000			Cs ₂ ZrO ₃	4000		
Cs ₂ MoO ₄	4000			Mo	9330	2890	4885	Cs ₂ Zr ₂ O ₅	4000		
Ba(OH) ₂	2180	351	1053	MoO ₂	6470			Cs ₂ Zr ₃ O ₇	4000		
BaO	5720	2196	2273	MoO ₃	4692	1068		Cs ₂ Te	4000		
BaI ₂	5150	1013		Ag	9345	1235	2485	Cs ₂ TeO ₃	4000		
Ba	3325	1002	1910	Ag ₂ Te	8500	1228		Cs ₂ Te ₂ O ₅	4000		
BaTe	5130			B	2340	2573	3931	Cs ₂ Te ₄ O ₉	4000		
BaZrO ₃	4000			B ₂ O ₃	1812	723		Cs ₂ TeO ₄	4000		
BaUO ₄	4000			CsBO ₂	4000			Cs ₂ Te ₄ O ₁₂	4000		
BaMoO ₄	4650	1753		HBO ₂	2486	509		Cs ₂ Cr ₂ O ₇	4000		

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Table 8.6: Density, Melting Point, and Boiling Point for the Condensed-Phase Species

Name	ρ (kg/ m ³)	T _M (K)	T _B (K)	Name	ρ (kg/ m ³)	T _M (K)	T _B (K)	Name	ρ (kg/ m ³)	T _M (K)	T _B (K)
Sr(OH) ₂	3625	648	983	H ₃ BO ₃	1435			Cs ₂ CrO ₄	4237		
SrO	4700	2703	3273	ZrB ₂	6085	3273		Cs ₃ CrO ₄	4000		
SrI ₂	2549	788		Cd	7996	594	1038	Cs ₄ CrO ₄	4000		
Sr	2375	1657	2375	CdO	8150			BaH ₂	4210		
SrUO ₄	4000			CdTe	6200	1314		SrH ₂	3720		
SrZrO ₃	4000			Cr	6460	2130	2945	ZrI ₄	4000	772	
SrMoO ₄	4540			Cr ₂ O ₃	5210	2708	4273	ZrTe ₂	4000		
ZrO ₂	5890	2973	5273	CrTe	4000			Tel ₄	5403	553	
Zr	5800	2125	4650	In	7032	429	2353	H ₂ TeO ₄	4000		
Sn	6973	505	2543	In ₂ O ₃	7179			UO ₃ ·2H ₂ O	4000		
SnO	6446	1353		InTe	6290	969		Fe(OH) ₂	3400		
SnO ₂	6950			Mn	6430	1517	2235	Mol ₄	4000		
SnI ₂	5285	593	990	MnO	5430			Mol ₃	4000		
SnTe	6480	1053		Mn ₃ O ₄	4856	1978		Mol ₂	5278		
Te	5797	723	1263	MnTe	4000			AgI	6010	831	1779
TeO ₂	5670	1006	1518	MnTe ₂	4000			CdI ₂	5670	660	1069
UO ₂	10960	2773		Ni	7780	1726	3005	CrI ₂	5196	1129	
U	17907	1406	4018	NiO	6670	2263		InI	5310	624	986
U ₄ O ₉	4000			Ru	10900	2583	4173	Nil ₂	5834	1070	
U ₃ O ₈	8300			RuO ₂	6970			Ru ₃ U	4000		
UO ₃	7290			Sb	6483	904	1908	RuTe ₂	4000		
Fe	7035	1808	3023	Sb ₂ O ₃	5200	929					

8.7 Structural Properties

The following data are used in the decay heating model for structures and deposited films, as described in Subsection 3.6.3. Deposited film density is calculated in the same way as the density for aerosol particles, as described in Subsection 5.2.2. Property val-

Thermochemical and Physical Data

ues for oxidized Inconel and stainless steel are taken to be identical to the ones for the unoxidized materials because, by assumption, only a thin surface layer is oxidized; the underlying structure is identical in both cases. The deposited film is assigned the characteristics of Fe_2O_3 .

Table 8.7: Mechanical and Thermal Properties of Structural Materials

Structure Identification Number	Material	Density (kg/m ³)	Heat Capacity (J/kgK)	Thermal Conductivity (W/mK)	Reference
0	Inert (ZrO_2)	5700	570	1.7	Hohorst, 1990
1	Zircaloy-4	6550	340	18	Hohorst, 1990
2	Inconel-600	8420	900	15	Schmidt et al., 1991
3	304 Stainless steel	7930	800	15	Schmidt et al., 1991
4	Oxidized Inconel-600	8420	900	15	Schmidt et al., 1991
5	Oxidized stainless steel	7930	800	15	Schmidt et al., 1991
6	Zirconia	5700	570	1.7	Hohorst, 1990
	Deposited film (Fe_2O_3)	Calc.	950	3.4	Hohorst, 1990

Part IV: Numerical Methods

9.0 Numerical Algorithms Used in VICTORIA

9.1 General Time-Step Strategy

At each time step, the models described in Chapters 1 through 5 are executed sequentially in the following order:

1. release of elements in control rod alloy (Section 2.4),
2. release of fuel elements (Sections 2.1, 2.2, 2.5, and 2.6),
3. bulk gas transport (Sections 3.3 and 3.5),
4. aerosol agglomeration and deposition (Sections 5.3, 5.5 and 5.6),
5. decay heat on surfaces (Section 3.6),
6. structure heatup (Section 3.6), and
7. equilibrium and nonequilibrium chemistry (Sections 4.1 through 4.3).

Details of the nature of these models are given in the referenced sections. Further details are set out in this chapter on the numerical methods used for models that involve partial differential equations. In addition, details on the numerical methods used to solve for general thermochemical equilibrium and frozen chemistry are given.

9.2 Transport in the Fuel

The general equation used to solve for diffusion and advection of gases in the fuel pores, fuel/clad gap, cladding, and the external boundary layer is given by Equation (2.30), which is

$$\alpha \frac{\partial C(i)}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left[r \beta_r D(i) \frac{\partial C(i)}{\partial r} - r C(i) u \right] + \frac{\partial}{\partial z} \left[\beta_z D(i) \frac{\partial C(i)}{\partial z} - C(i) v \right] \quad (9.1)$$

where

- α = total porosity (dimensionless)
- t = time (s)
- $C(i)$ = molar concentration of species i (kg-mol/m³)
- r = radial coordinate (m)
- z = axial coordinate (m)
- β_r = interconnected porosity in the radial dimension (dimensionless)
- β_z = interconnected porosity in the axial dimension (dimensionless)
- $D(i)$ = gaseous diffusivity of species i (m²/s)
- u = gas velocity in the radial dimension (m/s)
- v = gas velocity in the axial dimension (m/s)

Numerical Algorithms Used in VICTORIA

The sources of volatile fission products from the fuel grains are not included in Equation (9.1); instead, these sources are included in the initial condition at each time step. Default values for total porosity, α , and interconnected porosity, β , in the fuel pellets, gap, and cladding are described in Chapter 2; modification of these defaults is discussed in Chapter 6. Both total and interconnected porosities are equal to unity in the external boundary layer and there are no options to modify these values in the input file. The models and correlations used to define the gaseous diffusivities, $D(i)$, are also described in Chapter 2.

The initial and boundary conditions on Equation (9.1) are given in Chapter 2 to be

$$C(i)|_{t=t_0} = C_0(i, r, z) \text{ for } 0 \leq r \leq d/2 + t_{\text{gap}} + t_{\text{clad}} + \delta \quad (9.2)$$

$$\frac{\partial}{\partial r} C(i)|_{r=0} = 0 \text{ for } t > t_0 \quad (9.3)$$

$$\frac{\partial}{\partial r} C(i) \Big|_{r=d/2+t_{\text{gap}}+t_{\text{clad}}+\delta} = 0 \text{ for } t > t_0 \quad (9.4)$$

$$\frac{\partial}{\partial z} C(i) \Big|_{z=0} = 0 \text{ for } t > t_0 \quad (9.5)$$

$$\frac{\partial}{\partial z} C(i) \Big|_{z=L} = 0 \text{ for } t > t_0 \quad (9.6)$$

where

t_0	=	initial time (s)
$C_0(i, r, z)$	=	initial concentration of species i at radial position r and axial position z (kg-mol/m ³)
d	=	fuel pellet diameter (m)
t_{gap}	=	gap thickness (m)
t_{clad}	=	cladding thickness (m)
δ	=	external boundary layer thickness (m)
L	=	height of fuel rod (m)

The equations that determine the axial and radial gas velocities are given in (2.34) and (2.35), which are

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$$u = -\frac{\kappa_r}{\mu} \frac{\partial P}{\partial r} \quad (9.7)$$

$$v = -\frac{\kappa_z}{\mu} \frac{\partial P}{\partial z} \quad (9.8)$$

where

κ_r	= permeability in the radial dimension (m ²)
κ_z	= permeability in the axial dimension (m ²)
μ	= dynamic viscosity of the gas phase (kg/m·s)
P	= total gas pressure (Pa)

Total gas pressure is calculated by summing the partial gas pressures, as shown in Equation (2.21).

Equation (9.1) is solved using a multistep process. First, the radial flow of gases caused by pressure gradients is calculated from the following equation, which is simply an expression of Richards equation for a compressible gas in a radial coordinate system (Freeze and Cherry, 1979):

$$\alpha \frac{\partial P}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left[r P \frac{\kappa_r}{\mu} \frac{\partial P}{\partial r} \right] \quad (9.9)$$

subject to initial and boundary conditions

$$P|_{t=t_0} = P_0(r, z) \text{ for } 0 \leq r \leq d/2 + t_{\text{gap}} + t_{\text{clad}} + \delta \quad (9.10)$$

$$\left. \frac{\partial P}{\partial r} \right|_{r=0} = 0 \text{ for } t > t_0 \quad (9.11)$$

$$\left. \frac{\partial P}{\partial r} \right|_{r=d/2+t_{\text{gap}}+t_{\text{clad}}+\delta} = 0 \text{ for } t > t_0 \quad (9.12)$$

Equation (9.9) is obtained by summing Equation (9.1) over all of the gaseous species and by assuming that the net rates of diffusion and axial advection are negligible. (These terms are considered below.) The numerical procedure for solving Equation (9.9) is based on the finite-difference method. The discretized form of Equation (9.9) is

Numerical Algorithms Used in VICTORIA

$$\begin{aligned}
 & \frac{\alpha(t)|_{m,n}}{\Delta t} [P(t + \Delta t) - P(t)]_{m,n} \\
 &= \frac{1}{r_{m,n}} \left[rP(t + \Delta t) \frac{\kappa_r}{\mu} \right]_{m+1/2,n} \frac{P(t + \Delta t)|_{m+1,n} - P(t + \Delta t)|_{m,n}}{(r_{m+1/2} - r_{m-1/2})(r_{m+1,n} - r_{m,n})} \\
 & - \frac{1}{r_{m,n}} \left[rP(t + \Delta t) \frac{\kappa_r}{\mu} \right]_{m-1/2,n} \frac{P(t + \Delta t)|_{m,n} - P(t + \Delta t)|_{m-1,n}}{(r_{m+1/2} - r_{m-1/2})(r_{m,n} - r_{m-1,n})} \quad (9.13)
 \end{aligned}$$

where the subscripts m and n refer to the radial and axial subnode numbers, respectively; values at $m + 1/2$ are evaluated at the boundary between radial nodes m and $m + 1$; and values at $m - 1/2$ are evaluated at the boundary between radial nodes $m - 1$ and m .

Nodalization of a fuel rod is illustrated in Figure 9.1 for a case where the pellets contain two radial subnodes and the fuel rods contain three axial levels. The total number of radial subnodes is five, including one for the fuel/clad gap, one for the cladding, and one for the external boundary layer. Thus the total number of subnodes representing the fuel rod and its boundary layer is fifteen.

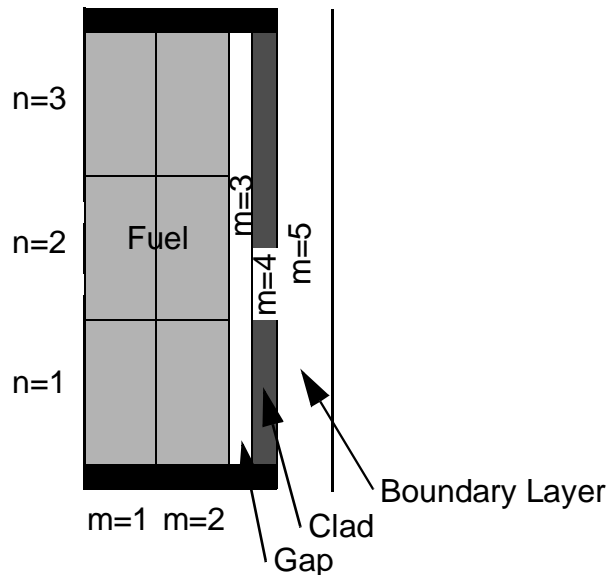


Figure 9.1. Illustration of a nodalization of a fuel rod.

The system of equations represented by Equation (9.10) (one equation for each value of m and n) is nonlinear in the unknown total gas pressure, $P(t + \Delta t)$, so an iterative technique, the Newton-Raphson procedure, is employed to solve the system. To implement the Newton-Raphson procedure, Equation (9.10) is rewritten in residual form as follows:

Numerical Algorithms Used in VICTORIA

$$\begin{aligned}
 R_{m,n} = & \frac{\alpha(t)|_{m,n}}{\Delta t} [P(t + \Delta t) - P(t)]_{m,n} \\
 & - \frac{1}{r_{m,n}} \left[r P(t + \Delta t) \frac{\kappa_r}{\mu} \right]_{m+1/2,n} \frac{P(t + \Delta t)|_{m+1,n} - P(t + \Delta t)|_{m,n}}{(r_{m+1/2} - r_{m-1/2})(r_{m+1,n} - r_{m,n})} \\
 & + \frac{1}{r_{m,n}} \left[r P(t + \Delta t) \frac{\kappa_r}{\mu} \right]_{m-1/2,n} \frac{P(t + \Delta t)|_{m,n} - P(t + \Delta t)|_{m-1,n}}{(r_{m+1/2} - r_{m-1/2})(r_{m,n} - r_{m-1,n})}
 \end{aligned} \quad (9.14)$$

where

$R_{m,n}$ = residual for the equation representing subnode m,n (dimensionless)

When the system of equations is solved, each of the residuals should be within some small tolerance of zero. To determine the values of pressure, each of the residual equations is linearized in the unknown gas pressure, $P(t + \Delta t)$, as follows:

$$\frac{\partial R_{m,n}}{\partial P(t + \Delta t)|_{m-1,n}} = -\frac{1}{r_{m,n}} \left[r \frac{\kappa_r}{\mu} \right]_{m-1/2,n} \frac{P(t + \Delta t)|_{m-1,n}}{(r_{m+1/2} - r_{m-1/2})(r_{m,n} - r_{m-1,n})} \quad (9.15)$$

$$\begin{aligned}
 \frac{\partial R_{m,n}}{\partial P(t + \Delta t)|_{m,n}} = & \frac{\alpha(t)|_{m,n}}{\Delta t} + \frac{1}{r_{m,n}(r_{m+1/2} - r_{m-1/2})} \left\{ \left[r \frac{\kappa_r}{\mu} \right]_{m+1/2,n} \left[\frac{P(t + \Delta t)|_{m,n}}{r_{m+1,n} - r_{m,n}} \right] \right. \\
 & \left. + \left[r \frac{\kappa_r}{\mu} \right]_{m-1/2,n} \left[\frac{P(t + \Delta t)|_{m,n}}{r_{m,n} - r_{m-1,n}} \right] \right\}
 \end{aligned} \quad (9.16)$$

$$\frac{\partial R_{m,n}}{\partial P(t + \Delta t)|_{m+1,n}} = -\frac{1}{r_{m,n}} \left[r \frac{\kappa_r}{\mu} \right]_{m+1/2,n} \frac{P(t + \Delta t)|_{m+1,n}}{(r_{m+1/2} - r_{m-1/2})(r_{m+1,n} - r_{m,n})} \quad (9.17)$$

The linear set of equations (one for each value of m and n)

$$\begin{aligned}
 0 = & R_{m,n} + \frac{\partial R_{m,n}}{\partial P(t + \Delta t)|_{m-1,n}} \delta P(t + \Delta t)|_{m-1,n} + \frac{\partial R_{m,n}}{\partial P(t + \Delta t)|_{m,n}} \delta P(t + \Delta t)|_{m,n} \\
 & + \frac{\partial R_{m,n}}{\partial P(t + \Delta t)|_{m+1,n}} \delta P(t + \Delta t)|_{m+1,n}
 \end{aligned} \quad (9.18)$$

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is then solved to determine each of the corrections to the nodal pressures, $\delta P(t + \Delta t)|_{m,n}$. The iteration process is continued until the following criterion is satisfied:

$$\frac{\text{rms}}{P_{\max}} < 10^{-6} \quad (9.19)$$

where

rms = root mean square of the changes to the nodal pressures (Pa)
 P_{\max} = maximum pressure in any of the nodes (Pa)

Once the radial velocities are determined, the axial velocities are calculated in exactly the same fashion, beginning with the equation

$$\alpha \frac{\partial P}{\partial t} = \frac{\partial}{\partial z} \left[P \frac{\kappa_z}{\mu} \frac{\partial P}{\partial z} \right] \quad (9.20)$$

subject to initial and boundary conditions

$$P|_{t=t_0} = P_0(r, z) \text{ for } 0 \leq z \leq L \quad (9.21)$$

$$\left. \frac{\partial P}{\partial z} \right|_{z=0} = 0 \text{ for } t > t_0 \quad (9.22)$$

$$\left. \frac{\partial P}{\partial z} \right|_{z=L} = 0 \text{ for } t > t_0 \quad (9.23)$$

where the initial pressure at each time step, $P_0(r, z)$, is the result of the solution to Equations (9.9) through (9.12).

The algorithm to solve Equations (9.20) through (9.23) is essentially identical to the one described above. The pressure profile obtained is used to determine the radial and axial velocities from Equations (9.7) and (9.8), which are needed to solve Equation (9.1).

The solution algorithm for Equation (9.1) is also based on the finite-difference method. The discretized form of Equation (9.1) is the following:

Numerical Algorithms Used in VICTORIA

$$\begin{aligned}
 & \frac{\alpha(t)|_{m,n}}{\Delta t} [C(i, t + \Delta t) - C(i, t)]_{m,n} \\
 &= \frac{1}{r_{m,n}} [r\beta_r D(i)]_{m+1/2,n} \frac{C(i, t + \Delta t)|_{m+1,n} - C(i, t + \Delta t)|_{m,n}}{(r_{m+1/2,n} - r_{m-1/2,n})(r_{m+1,n} - r_{m,n})} - \frac{[ruC(i, t + \Delta t)]_{m+1/2,n}}{r_{m+1/2,n} - r_{m-1/2,n}} \\
 &- \frac{1}{r_{m,n}} \left\{ [r\beta_r D(i)]_{m-1/2,n} \frac{C(i, t + \Delta t)|_{m,n} - C(i, t + \Delta t)|_{m-1,n}}{(r_{m+1/2,n} - r_{m-1/2,n})(r_{m,n} - r_{m-1,n})} - \frac{[ruC(i, t + \Delta t)]_{m-1/2,n}}{r_{m+1/2,n} - r_{m-1/2,n}} \right\} \\
 &+ [\beta_z D(i)]_{m,n+1/2} \frac{C(i, t + \Delta t)|_{m,n+1} - C(i, t + \Delta t)|_{m,n}}{(z_{m,n+1/2} - z_{m,n-1/2})(z_{m,n+1} - z_{m,n})} - \frac{[vC(i, t + \Delta t)]_{m,n+1/2}}{z_{m,n+1/2} - z_{m,n-1/2}} \\
 &- [\beta_z D(i)]_{m,n-1/2} \frac{C(i, t + \Delta t)|_{m,n} - C(i, t + \Delta t)|_{m,n-1}}{(z_{m,n+1/2} - z_{m,n-1/2})(z_{m,n} - z_{m,n-1})} + \frac{[vC(i, t + \Delta t)]_{m,n-1/2}}{z_{m,n+1/2} - z_{m,n-1/2}} \quad (9.24)
 \end{aligned}$$

Because equations in the set represented by (9.24) are already linear in the unknown concentrations, $C(i, t + \Delta t)|_{m,n}$, a standard linear solution algorithm, a band solver, is employed to determine the concentrations for each of the subnodes.

9.3 Bulk Gas Transport

Transport of vapors within the RV and RCS is governed by Equation (3.10), which is

$$\frac{\partial}{\partial t} c(i) = \frac{1}{A_r} \frac{\partial}{\partial r} \left[A_r D(i) \frac{\partial}{\partial r} c(i) - A_r u c(i) \right] + \frac{1}{A_z} \frac{\partial}{\partial z} \left[A_z D(i) \frac{\partial}{\partial z} c(i) - A_z v c(i) \right] + \frac{S_F + S_C + S_S}{V_B} \quad (9.25)$$

and is subject to the following initial and boundary conditions:

$$c(i) = c_0(i) \text{ when } t = t_0 \quad (9.26)$$

$$\frac{\partial}{\partial t} c(i) = 0 \text{ on all domain boundaries} \quad (9.27)$$

where

- t = time (s)
- $c(i)$ = mass concentration of species i (kg/m³)
- r = radial coordinate (m)
- z = axial coordinate (m)
- A_r = area for flow and diffusion in radial dimension (m²)

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- A_z = area for flow and diffusion in axial dimension (m²)
 $D(i)$ = diffusivity of species i in the gas mixture (m²/s)
 u = radial component of velocity (m/s)
 v = axial component of velocity (m/s)
 S_F = source of mass from fuel layer (kg/s)
 S_C = source of mass from control rod layer (kg/s)
 S_S = source of mass from structural surface layer (kg/s)
 V_B = volume of the bulk gas subregion (m³)
 0 = subscript referring to initial condition

The three source rate terms, S_F , S_C , and S_S , are defined in Equations (3.13) through (3.15) and are nearly linear in the unknown concentrations, $c(i)$. Equation (9.25) is solved using the upwind variant of the finite-difference method. The discretized form of (9.25) is the following:

$$\begin{aligned}
 & \frac{c(i, t + \Delta t) - c(i, t)}{\Delta t} \\
 &= \frac{1}{A_r|_{m,n}} \left\{ [A_r D(i)]_{m+1/2,n} \frac{C(i, t + \Delta t)|_{m+1,n} - C(i, t + \Delta t)|_{m,n}}{(r_{m+1/2,n} - r_{m-1/2,n})(r_{m+1,n} - r_{m,n})} \right. \\
 & \quad \left. - \frac{(A_r u f)_{m+1/2,n} [C(i, t + \Delta t)]_{m,n} + (A_r u g)_{m+1/2,n} [C(i, t + \Delta t)]_{m+1,n}}{r_{m+1/2,n} - r_{m-1/2,n}} \right\} \\
 & - \frac{1}{A_r|_{m,n}} \left\{ [A_r D(i)]_{m-1/2,n} \frac{C(i, t + \Delta t)|_{m,n} - C(i, t + \Delta t)|_{m-1,n}}{(r_{m+1/2,n} - r_{m-1/2,n})(r_{m,n} - r_{m-1,n})} \right. \\
 & \quad \left. - \frac{(A_r u f)_{m-1/2,n} [C(i, t + \Delta t)]_{m-1,n} + (A_r u g)_{m-1/2,n} [C(i, t + \Delta t)]_{m,n}}{r_{m+1/2,n} - r_{m-1/2,n}} \right\} \\
 & + \frac{1}{A_z|_{m,n}} \left\{ [A_z D(i)]_{m,n+1/2} \frac{C(i, t + \Delta t)|_{m,n+1} - C(i, t + \Delta t)|_{m,n}}{(z_{m,n+1/2} - z_{m,n-1/2})(z_{m,n+1} - z_{m,n})} \right. \\
 & \quad \left. - \frac{(A_z v f)|_{m,n+1/2} [C(i, t + \Delta t)]_{m,n} + (A_z v g)|_{m,n+1/2} [C(i, t + \Delta t)]_{m,n+1}}{z_{m,n+1/2} - z_{m,n-1/2}} \right\} \\
 & + \frac{1}{A_z|_{m,n}} \left\{ [A_z D(i)]_{m,n-1/2} \frac{C(i, t + \Delta t)|_{m,n} - C(i, t + \Delta t)|_{m,n-1}}{(z_{m,n+1/2} - z_{m,n-1/2})(z_{m,n} - z_{m,n-1})} \right. \\
 & \quad \left. - \frac{(A_z v f)|_{m,n-1/2} [C(i, t + \Delta t)]_{m,n-1} + (A_z v g)|_{m,n-1/2} [C(i, t + \Delta t)]_{m,n}}{z_{m,n+1/2} - z_{m,n-1/2}} \right\}
 \end{aligned}$$

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$$+ \left[\frac{S_F + S_C + S_S}{V_B} \right]_{m,n} \quad (9.28)$$

where

$f = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ if $\begin{pmatrix} u \geq 0 \\ u < 0 \end{pmatrix}$ in the radial terms;

$f = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ if $\begin{pmatrix} v \geq 0 \\ v < 0 \end{pmatrix}$ in the axial terms; and

$g = 1 - f$

9.4 Aerosol Agglomeration and Deposition

The equation that governs aerosol agglomeration and deposition is given in (5.19), which is as follows:

$$\frac{\partial}{\partial t} N(m) = \frac{1}{2} \int_0^m \Phi(\omega, m - \omega) N(\omega) N(m - \omega) d\omega - N(m) \int_0^\infty \Phi(\omega, m) N(\omega) d\omega - R(m) + S(m) \quad (9.29)$$

where

- $N(m)$ = aerosol number concentration of particles of mass m ($1/m^3$)
- $\Phi(\omega, m)$ = agglomeration kernel ($m^3/kg \cdot s$), i.e., a measure of the rate at which particles of mass ω agglomerate with particles of mass m
- m, ω = mass of an aerosol particle (kg)
- $R(m)$ = volumetric removal rate of particles of size m due to deposition ($1/m^3 \cdot s$)
- $S(m)$ = volumetric source rate of particles of size m ($1/m^3 \cdot s$)

The terms in Equation (9.29) are defined in Chapter 5. The numerical treatment of (9.29) follows the collocation finite element method, as explained in the CHARM manual (Wheatley, 1988). A brief summary of the numerical method is given here. First, Equation (9.29) is transformed using the relationship $Y(m) = mN(m)$ to obtain the following equation:

$$\frac{\partial}{\partial t} Y(m) = \int_0^{\ln m} \Phi(\omega, m - \omega) Y(\omega) Y(m - \omega) d \ln \omega - Y(m) \int_0^\infty \Phi(\omega, m) Y(\omega) d \ln \omega - mR(m) + mS(m) \quad (9.30)$$

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The variable $Y(m)$ has the physical meaning of aerosol concentration in units of kg/m^3 for particles of mass m . Thus, $Y(m)$ is the unknown aerosol mass concentration distribution. Following the finite-element method, $Y(m)$ is expanded in a set of basis functions as follows:

$$Y(m) = \sum_i Y_j g_j(\ln m) \quad (9.31)$$

where

Y_j = a set of time-dependent coefficients that are to be determined (kg/m^3)
 $g_j(\ln m)$ = a set of finite-element basis functions, which depend only on the natural logarithm of aerosol particle mass, $\ln m$

The basis functions, g_j , are chosen in keeping with the collocation finite-element method to be the Kronecker delta functions, as defined in the following relationship:

$$g_j(x_k) = \delta_{jk} \quad (9.32)$$

where

$$x_k = \ln m_k$$

and the values of x_k are defined as follows:

$$x_k = x_1 + (k - 1)\Delta x \quad (9.33)$$

where

x_1 = the natural logarithm of the smallest aerosol mass to be represented in the numerical representation of the aerosol size distribution (kg), as specified in the VICTORIA input file and discussed in Chapter 6.
 Δx = the logarithmic spacing between aerosol masses in the representation of the aerosol mass distribution (kg), as specified in the VICTORIA input file and discussed in Chapter 6.

With these choices, Equation (9.30) becomes

$$\frac{dY_i}{dt} = \sum_j \sum_k P_{jk}^i \Phi_{jk} Y_j Y_k - \Delta x Y_i \sum_j \Phi_{ij} Y_j - m_i (R_i - S_i) \quad (9.34)$$

where

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$$P_{jk}^i = n_{jk} \int_0^{x_i} g_j(x) g_k(x_i - x) dx \quad (9.35)$$

Φ_{jk} = shorthand for $\Phi(m_j, m_k)$
 R_i = shorthand for $R(m_i)$
 S_i = shorthand for $S(m_i)$

and n_{jk} are defined in order to conserve mass, as explained in Wheatley (1988). Equation (9.34) represents a set of ordinary differential equations. The number of equations in the set is determined by the user-specified range of aerosol masses to be represented and the spacing between aerosol masses, as specified by Equation (9.33). These ordinary differential equations are solved using the library routine, DEBDF, which was written by Shampine and Watts (1979).

9.5 General Equilibrium Thermochemistry

The technique used in VICTORIA to determine the conditions at thermodynamic equilibrium is first illustrated for a simple system containing only the elements Eu and O; then it is generalized to the complete system of 26 elements in the VICTORIA database. The Eu-O system is especially useful for understanding the VICTORIA methodology because vaporization of $\text{Eu}_2\text{O}_3(c)$ is noncongruent and so does not obey Raoult's law.

9.5.1 Illustration for Eu and O

There are nine species in the VICTORIA thermochemical database that are composed only of Eu and O:

1. $\text{O}(v)$
2. $\text{O}_2(v)$
3. $\text{Eu}(v)$
4. $\text{EuO}(v)$
5. $\text{Eu}_2\text{O}(v)$
6. $\text{Eu}_2\text{O}_2(v)$
7. $\text{Eu}(c)$
8. $\text{EuO}(c)$
9. $\text{Eu}_2\text{O}_3(c)$

For a fixed number of moles of Eu and O contained in a fixed total volume, V , conservation of the number of moles of each element per unit volume is expressed as follows:

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$$\frac{n(\text{Eu})}{V} = C[\text{Eu}(v)] + C[\text{EuO}(v)] + 2C[\text{Eu}_2\text{O}(v)] + 2C[\text{Eu}_2\text{O}_2(v)] + C[\text{Eu}(c)] + C[\text{EuO}(c)] + 2C[\text{Eu}_2\text{O}_3(c)] \quad (9.36)$$

$$\frac{n(\text{O})}{V} = C[\text{O}(v)] + 2C[\text{O}_2(v)] + C[\text{EuO}(v)] + C[\text{Eu}_2\text{O}(v)] + 2C[\text{Eu}_2\text{O}_2(v)] + C[\text{EuO}(c)] + 3C[\text{Eu}_2\text{O}_3(c)] \quad (9.37)$$

where the following definitions apply:

n	=	number of moles of an element
V	=	total volume
C	=	moles of a species per total volume, i.e., molar concentration
v	=	vapor-phase species
c	=	condensed-phase species

Since the quantities on the left-hand side of Equations (9.36) and (9.37) are fixed, these two equations contain nine unknowns, namely, the concentrations of the nine species listed above. The number of unknowns can be reduced to three by applying the mass action laws for the reactions of formation for each species from the vapor-phase elements, which are

$$2\text{O}(v) = \text{O}_2(v) \quad (9.38)$$

$$\text{Eu}(v) + \text{O}(v) = \text{EuO}(v) \quad (9.39)$$

$$2\text{Eu}(v) + \text{O}(v) = \text{Eu}_2\text{O}(v) \quad (9.40)$$

$$2\text{Eu}(v) + 2\text{O}(v) = \text{Eu}_2\text{O}_2(v) \quad (9.41)$$

$$\text{Eu}(v) = \text{Eu}(c) \quad (9.42)$$

$$\text{Eu}(v) + \text{O}(v) = \text{EuO}(c) \quad (9.43)$$

$$2\text{Eu}(v) + 3\text{O}(v) = \text{Eu}_2\text{O}_3(c) \quad (9.44)$$

The mass action laws for Equations (9.38) through (9.44) are given in Equations (9.45) through (9.51).

$$p(\text{O}_2) = K_3 p^2(\text{O}) \quad (9.45)$$

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$$p(\text{EuO}) = K_4 p(\text{Eu}) p(\text{O}) \quad (9.46)$$

$$p(\text{Eu}_2\text{O}) = K_5 p^2(\text{Eu}) p(\text{O}) \quad (9.47)$$

$$p(\text{Eu}_2\text{O}_2) = K_6 p^2(\text{Eu}) p^2(\text{O}) \quad (9.48)$$

$$x(\text{Eu}) = K_7 p(\text{Eu}) \quad (9.49)$$

$$x(\text{EuO}) = K_8 p(\text{Eu}) p(\text{O}) \quad (9.50)$$

$$x(\text{Eu}_2\text{O}_3) = K_9 p^2(\text{Eu}) p^3(\text{O}) \quad (9.51)$$

where the following definitions apply:

- p = partial pressure of a vapor-phase species, which for an ideal gas is related to concentration by $p = CRT$, which implicitly assumes that the gas volume is approximately the same as the total volume
- R = gas constant
- T = absolute temperature
- x = mole fraction of a condensed-phase species, which is related to concentration by $x(i) = C(i)/C_C$
- C_C = the total concentration of condensed-phase species, $\sum_{i \in C} C(j)$, where the summation is over the condensed-phase species
- K = equilibrium constant, which is defined as $K_i = \exp(-\Delta G_i/RT)$, where the subscript refers to the equation number for the reactions given above
- ΔG_i = the change in Gibbs free energy associated with reaction i

By using Equations (9.38) through (9.44) and the relationships between partial pressure, mole fraction, and concentration, each of the other unknown concentrations in Equations (1) and (2) can be eliminated in favor of $C[\text{Eu}(v)]$, $C[\text{O}(v)]$, and C_C . The resulting equations are

$$\begin{aligned} \frac{n(\text{Eu})}{V} = & C[\text{Eu}(v)] + K_4(RT)^2 C[\text{Eu}(v)] C[\text{O}(v)] / (RT) \\ & + \{ 2K_5(RT)^3 C^2[\text{Eu}(v)] C[\text{O}(v)] + 2K_6(RT)^4 C^2[\text{Eu}(v)] C^2[\text{O}(v)] \} / RT \\ & + \{ K_7 RTC[\text{Eu}(v)] + K_8(RT)^2 C[\text{Eu}(v)] C[\text{O}(v)] + 2K_9(RT)^5 C^2[\text{Eu}(v)] C^3[\text{O}(v)] \\ & + 2K_9(RT)^5 C^2[\text{Eu}(v)] C^3[\text{O}(v)] \} \times C_C \end{aligned} \quad (9.52)$$

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$$\begin{aligned} \frac{n(O)}{V} = & C[O(v)] + \{2K_3(RT)^2 C^2[O(v)] + K_4(RT)^2 C[Eu(v)]C[O(v)]\}/(RT) \\ & + \{K_5(RT)^3 C^2[Eu(v)]C[O(v)] + 2K_6(RT)^4 C^2[Eu(v)]C^2[O(v)]\}/(RT) \\ & + \{K_8(RT)^2 C[Eu(v)]C[O(v)] + 3K_9(RT)^5 C^2[Eu(v)]C^3[O(v)]\} \times C_C \end{aligned} \quad (9.53)$$

A third equation is needed in order to specify a unique solution. This equation is the requirement that the mole fractions of the condensed-phase species sum to unity.

$$\begin{aligned} 1 = & x(Eu) + x(EuO) + x(Eu_2O_3) \\ = & K_7 RTC[Eu(v)] + K_8(RT)^2 C[Eu(v)]C[O(v)] + K_9(RT)^5 C^2[Eu(v)]C^3[O(v)] \end{aligned} \quad (9.54)$$

This set of three nonlinear equations, (9.52) through (9.54), are solved iteratively for the three unknown concentrations, $C[Eu(v)]$, $C[O(v)]$, and C_C . The other concentrations are then determined from Equations (9.45) through (9.51).

Equations (9.52) through (9.54) are solved using a dual iterative technique that uses both cyclic Newton and Newton-Raphson methods. The cyclic Newton method consists of a sequential application of Newton's method for a single unknown. First, Newton's method is applied to Equation (9.52) to solve for $C[Eu(v)]$ given a fixed $C[O(v)]$ and C_C . Then the technique is applied to Equation (9.53) to solve for $C[O(v)]$ given a fixed $C[Eu(v)]$ and C_C . Finally, C_C is updated by summing the number of moles of condensed-phase species in the new solution. This is done by summing the contributions following the second equal sign in Equation (9.54) and multiplying by the previous value of C_C . Until the solution has converged, the condensed-phase mole fractions will generally not sum to unity.

This process is repeated for a number of times (as specified by user input). If convergence has not been attained, the Newton-Raphson method is applied once to solve simultaneously for $C[Eu(v)]$ and $C[O(v)]$. The number of moles of condensed-phase species, C_C , is then recalculated in the same way as in the cyclic Newton process. After this, the cyclic Newton process is invoked again.

The two iteration methods are continued in this fashion until convergence is attained, as determined by a user-input convergence parameter. If the iterative technique fails to converge, an error message is printed out to warn the user.

9.5.2 Solution Technique

The above illustration can be generalized to a large set of species (288 in VICTORIA) composed of a smaller set of elements (26 in VICTORIA). The set of molar balance equations is written as

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$$\frac{n(i)}{V} = \sum_{j \in S} L_{ji} C(j) = \frac{1}{RT} \sum_{j \in G} L_{ji} p(j) + C_C \sum_{j \in C} L_{ji} x(j) \text{ for } i \in E \quad (9.55)$$

where the following definitions apply

- S = set of all species in the database, of which there are s
- G = the set of all gas-phase species in the database, of which there are g
- C = the set of all condensed-phase species in the database, of which there are $c = s - g$
- E = set of all elements in the database, of which there are e
- L_{ji} = number of moles of element i in one mole of species j

The quantity on the left-hand side of Equation (9.55) is known for each i , so this represents e equations in $s+1$ unknowns. For each gas-phase species, a mass action law can be written for its formation from the gas-phase elements as follows:

$$p(j) = C(j)RT = K_j \prod_{i \in E} p^{L_{ji}}(i) = K_j \prod_{i \in E} [C(i)RT]^{L_{ji}} \text{ for } j \in G \quad (9.56)$$

Similarly, for each condensed-phase species, a mass action law can be written for its formation from the gas-phase species as follows:

$$x(j) = \frac{C(j)}{C_C} = K_j \prod_{i \in E} p^{L_{ji}}(i) = K_j \prod_{i \in E} [C(i)RT]^{L_{ji}} \text{ for } j \in C \quad (9.57)$$

Finally, the mole fractions of the condensed-phase species must sum to unity.

$$1 = \sum_{j \in C} x(j) = \sum_{j \in C} K_j \left[\prod_{i \in E} [C(i)RT]^{L_{ji}} \right] \quad (9.58)$$

Using Equations (9.56) and (9.57), each of the other concentrations in Equation (55) can be eliminated in favor of the concentrations of the gas-phase elements and the total molar concentration of the condensed phase, C_C .

$$\frac{n(i)}{V} = \frac{1}{RT} \sum_{j \in G} L_{ji} K_j \prod_{k \in E} [C(k)RT]^{L_{jk}} + C_C \sum_{j \in C} L_{ji} K_j \prod_{k \in E} [C(k)RT]^{L_{jk}} \text{ for } i \in E \quad (9.59)$$

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The number of unknowns in Equations (9.58) and (9.59) is $e+1$, which is the same as the number of equations. These nonlinear equations are then solved iteratively for the $e+1$ unknowns using the same technique described in the illustration above. The other concentrations are then determined using Equations (9.56) and (9.57).

9.6 Frozen Chemistry

The frozen chemistry model is a simplification of the model for general thermochemical equilibrium described in the preceding subsection. In the frozen chemistry model, chemical interactions are not allowed; only change of phase is considered. Thus, the following equation must be satisfied for all species:

$$C_T(i) = C_G(i) + C_C(i) \quad (9.60)$$

where

- $C_T(i)$ = total concentration of a chemical species, i , in both the vapor and condensed phases (kg-mol/m³)
- $C_G(i)$ = concentration of a chemical species, i , in the vapor phase (kg-mol/m³)
- $C_C(i)$ = concentration of a chemical species, i , in the condensed phase (kg-mol/m³)

Here the volume basis for calculating concentration is taken to be the entire volume that contains both vapor and condensed phases. The equilibrium vapor-phase concentration is calculated from Raoult's and the ideal gas laws as follows:

$$C_G(i) = \frac{p(i)}{RT} = \frac{p'(i)x(i)}{RT} \quad (9.61)$$

where

- $p(i)$ = partial pressure of vapor species i (Pa)
- R = gas constant (kg·m²/s²·kg-mol)
- T = absolute temperature (K)
- $p'(i)$ = equilibrium vapor pressure of pure species i (Pa)
- $x(i)$ = mole fraction of species i in the condensed phase in which it is soluble (dimensionless)

The condensed-phase mole fraction is defined by the following equation:

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$$x(i) = \frac{C_C(i)}{\sum_{j \in C_i} C_C(j)} \quad (9.62)$$

where

C_i = set of condensed-phase species that are soluble in the same phase as species i (kg-mol/m³)

Substituting Equations (9.61) and (9.62) into (9.60) yields

$$C_T(i) - C_C(i) - \frac{p'(i)}{RT} \frac{C_C(i)}{\sum_{j \in C_i} C_C(j)} = R_i = 0 \quad (9.63)$$

where

R_i = residual equation for chemical species i , which is equal to zero when chemical equilibrium is attained (kg-mol/m³)

Equation (9.63) would be linear if it were not for the summation term in the denominator. Since it is nonlinear, the Newton-Raphson procedure is applied to obtain a solution. The Jacobian matrix is obtained by taking the derivatives of the residual equations with respect to each of the unknown concentrations.

$$\frac{\partial R_i}{\partial C_C(i)} = -1 - \frac{p'(i)}{RT} \left[\frac{1}{\sum_{j \in C_i} C_C(j)} - \frac{C_C(i)}{\left(\sum_{j \in C_i} C_C(j) \right)^2} \right] \quad (9.64)$$

$$\frac{\partial R_i}{\partial C_C(j)} = \frac{p'(i)}{RT} \left[\frac{C_C(i)}{\left(\sum_{k \in C_i} C_C(k) \right)^2} \right] \text{ for } i \neq j \quad (9.65)$$

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The Jacobian matrix is defined simply as

$$J_{ij} = \frac{\partial R_i}{\partial C_C(j)} \quad (9.66)$$

Finally, the Newton-Raphson iteration is implemented in the standard fashion:

$$R_i + \sum_j J_{ij} \delta[C_C(j)] = 0 \quad (9.67)$$

where

$\delta[C_C(j)]$ = correction to the concentration of condensed-phase species j (kg-mol/m³)

The system of equations is considered to have converged when the largest correction in concentration, on a relative basis, is less than 10^{-3} . In practice, convergence is usually achieved in three or four iterations.

10.0 References

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11.0 Nomenclature

Characters in parentheses following a definition indicate units of the variable; (dimensionless) indicates that the variable is dimensionless. Quantities in square brackets indicate a default code value.

11.1 Lower-Case Symbols

a	= actual or effective grain diameter (m)
a_{ij}	= the number of moles of element j in one mole of species i (dimensionless)
$c(i)$	= mass concentration of species i (kg/m ³)
$c_{\infty}(i)$	= mass concentration of species i in the gas far from an aerosol particle (kg/m ³)
$c_a(i)$	= mass concentration of species i in equilibrium with the surface of an aerosol particle (kg/m ³)
$c_F(i)$	= mass concentration of species i at fuel rod surface (kg/m ³)
d	= fuel pellet diameter (m)
\bar{d}_g	= geometric mean diameter (m)
\hat{d}_m	= mass median diameter of an equivalent spherical particle (m)
f	= Fanning friction factor (dimensionless)
$f(t,i)$	= integral fraction of initial inventory of fission product element i released at time t (dimensionless)
g	= gravitational acceleration (m/s ²)
h	= heat transfer coefficient (W/m ² ·K)
h_{dg}	= heat transfer coefficient between deposit and gas (W/m ² ·K)
h_{dS}	= heat transfer coefficient between deposit and structure (W/m ² ·K)
h_{SI}	= heat transfer coefficient between structure and insulation (W/m ² ·K)
k	= thermal conductivity (W/m·K)
$k(i)$	= thermal conductivity of species i (W/m·K)
k_a	= thermal conductivity of an aerosol particle (W/m·K)
k_g	= thermal conductivity of gas (W/m·K)
k_{ox}	= the kinetic coefficient of zirconium oxidation (kg ² /m ⁴ ·s)

Nomenclature

l_p	=	mean free path of a gas molecule (m)
m	=	mass of an aerosol particle (kg)
$m(j)$	=	inventory of fission product j in the fuel at the onset of the accident (kg)
\bar{m}_g	=	geometric mean mass (kg)
\hat{m}_m	=	mass median mass (kg)
$p(i)$	=	partial pressure of species i (Pa or atm.)
$p'(i)$	=	equilibrium vapor pressure of pure species i (Pa or atm.)
$q(j,t)$	=	decay power per mass of fission product element j as a function of time t (W/kg)
$\tilde{q}(j,t)$	=	the ratio of decay heat for fission product j to total operating power prior to scram as a function of time, t (dimensionless)
r	=	radial coordinate (m)
r_a	=	radius of aerosol particle (m)
$r_a(m)$	=	radius of aerosol particles with mass m (m)
r_m	=	radius of particle with mass m (m)
r_ω	=	radius of particle with mass ω (m)
t	=	time (s)
t_{clad}	=	cladding thickness (m)
t_{gap}	=	gap thickness (m)
t_o	=	time offset (s) [10]
t_0	=	initial time of calculation (s)
u	=	radial component of gas velocity (m/s)
u_b	=	deposition velocity induced by flow irregularities (m/s)
u_c	=	net deposition velocity at a ceiling surface (m/s)
u_d	=	deposition velocity for diffusion in a laminar flow (m/s)
u_f	=	net deposition velocity at a floor surface (m/s)
u_g	=	deposition velocity for gravitational settling (m/s)
u_t	=	deposition velocity in a turbulent flow field (m/s)
$u_{t,s}$	=	turbulent deposition velocity for submicron particles (m/s)
$u_{t,S}$	=	turbulent deposition velocity for supermicron particles (m/s)

Nomenclature

u_w	=	net deposition velocity at a wall surface (m/s)
u_T	=	thermophoretic deposition velocity (m/s)
v	=	axial component of gas velocity (m/s)
\tilde{v}	=	friction velocity (m/s)
v_a	=	axial velocity component of aerosol particle (m/s)
v_g	=	particle settling velocity (m/s)
$v_g(m)$	=	gravitational settling velocity of a particle of mass m (m/s)
v_d	=	vapor deposition velocity (m/s)
w	=	the mass of Zr consumed per unit surface area (kg/m ²)
x	=	excess oxygen in the fuel, as defined by UO_{2+x} (dimensionless)
$x(i)$	=	mole fraction of species i (kg/m ³)
x_{ox}	=	the mole fraction of zirconium in the cladding that is oxidized (dimensionless)
z	=	axial coordinate (m)

11.2 Upper-Case Symbols

A	=	surface area (m ²)
A_r	=	area for flow and diffusion in radial dimension (m ²)
A_z	=	area for flow and diffusion in axial dimension (m ²)
B	=	particle mobility (s/kg)
$B(m)$	=	mobility of particle of mass m (s/kg)
B_{St}	=	coefficient in Stokes mobility law (s/kg)
C	=	set of condensed-phase species in the VICTORIA database
$C(i)$	=	molar concentration of species i (kg-mol/m ³)
C_i	=	set of iodide condensed-phase species in the VICTORIA database
C_m	=	set of metallic condensed-phase species in the VICTORIA database, or momentum accommodation coefficient (dimensionless) [1.14]
C_o	=	set of oxidic condensed-phase species in the VICTORIA database
C_s	=	thermal slip coefficient (dimensionless) [1.17]
C_t	=	thermal accommodation coefficient (dimensionless) [2.18]
$C_G(0,i)$	=	uniform initial molar concentration of element i in fuel grains (kg-mol/m ³)

Nomenclature

$C_P(i)$	=	heat capacity of species i (W/kg·K)
$C_{P,dep}$	=	heat capacity of deposited film (W/kg·K)
$C_{P,S}$	=	heat capacity of structure (W/kg·K)
$C_S(i)$	=	minimum of the solubility of fission product i in fuel grains (kg-mol/m ³) and initial grain concentration, $C_G(0,i)$
C_n	=	Cunningham's slip correction factor (dimensionless)
$D(i)$	=	diffusivity of species i in a gas mixture (m ² /s)
$D(i,j)$	=	binary diffusion coefficient of gaseous species i diffusing through gaseous species j (m ² /s)
D_i	=	pipe diameter at the inlet of the sudden contraction (m)
$D_m(i)$	=	the diffusion coefficient of gaseous species i in a mixture of all other gaseous species (m ² /s)
D_o	=	pipe diameter at the outlet of the sudden contraction (m)
D_v	=	perpendicular spacing between vanes (m)
D_B	=	Brownian diffusivity (m ² /s)
D_H	=	hydraulic diameter (m)
$D_G(i)$	=	grain lattice diffusion coefficient for element i (m ² /s)
$D_0(i)$	=	preexponential coefficient for diffusion of species i (m ² /s)
E	=	the set of elements in the VICTORIA database
F	=	fractional rate of resuspension (1/s)
F_g	=	settling parameter (dimensionless)
$Fu(m, \omega)$	=	Fuchs factor for particles of mass m interacting with particles of mass ω (m ²)
$Fu_1(m, \omega)$	=	factor from kinetic theory, i.e., when particle size is less than the mean free path of a gas molecule (m ²)
$Fu_2(m, \omega)$	=	factor from diffusion theory, i.e., when particle size is greater than the mean free path of a gas molecule (m ²)
G	=	set of gaseous species in the VICTORIA database
$G(i)$	=	Gibbs free energy of species i (kg·m ² /s ² ·kg·mol·K)
H	=	measure of diffusive-to-convective transport (dimensionless)
H_V	=	height of a vortex tube (m)

Nomenclature

K	=	equilibrium coefficient (units vary)
$K(i)$	=	mass transfer coefficient for species i ($\text{kg}/\text{m}^2\cdot\text{s}$)
L	=	length over which deposition takes place (m)
L_{dg}	=	heat flux from the deposited film to the gas (W/m^2)
L_{dS}	=	heat flux from the deposited film to the structure (W/m^2)
L_{SI}	=	heat flux from the structure to the insulation or thermal boundary layer surrounding the structure (W/m^2)
$M(i)$	=	molecular mass of species i ($\text{kg}/\text{kg}\cdot\text{mol}$)
N	=	number of bends in a chevron-type steam dryer
$N(i)$	=	the number of atoms in a molecule of species i (dimensionless)
$N(m)$	=	aerosol number concentration of particles of mass m ($1/\text{m}^3$)
P	=	total gas pressure (Pa)
Q	=	total decay power per surface area (W/m^2)
Q_{Tot}	=	total operating power prior to reactor scram (W)
R	=	gas constant ($\text{kg}\cdot\text{m}^2/\text{s}^2\cdot\text{kg}\cdot\text{mol}$)
$R(m)$	=	volumetric removal rate of particles of size m due to deposition ($1/\text{m}^3\cdot\text{s}$)
R_d	=	radial coordinate of a particle that will just deposit on the vortex tube wall at the top of the vortex tube (m)
R_v	=	radius of the vortex tube (m)
S	=	set of all species in the VICTORIA database
$S(m)$	=	volumetric source rate of particles of size m ($1/\text{m}^3\cdot\text{s}$)
S_C	=	source of mass from control rod layer (kg/s)
$S_G(i)$	=	rate fission product release of element i from the fuel grains into the fuel pores ($\text{kg}\cdot\text{mol}/\text{m}^3\cdot\text{s}$)
S_F	=	source of mass from fuel layer (kg/s)
$S_P(i)$	=	rate fission product release of vapors containing element i from the fuel grains into the fuel pores ($\text{kg}\cdot\text{mol}/\text{m}^3\cdot\text{s}$)
S_S	=	source of mass from structural surface layer (kg/s)
T	=	absolute temperature (K)
T_{dep}	=	temperature of deposited film (K)

Nomenclature

T_{fail}	=	temperature at which cladding is predicted to fail, e.g., by balloon rupture (K)
T_{fr}	=	temperature at which fuel frothing begins (K) [2300]
T_g	=	gas temperature (K)
T_{melt}	=	melting temperature of cladding (K)
T_s	=	surface temperature of fuel rod, control rod, or structure (K)
T_I	=	outer surface temperature of insulation or ambient gas temperature outside of structure (K)
T_S	=	temperature of structure (K)
U	=	gas speed (m/s), $\sqrt{u^2 + v^2}$
V	=	volume of subregion (m^3)
V_B	=	volume of bulk gas subregion (m^3)
V_C	=	volume of control rod subregion (m^3)
V_F	=	volume of fuel layer subregion (m^3)
V_N	=	volume of node (m^3)
V_S	=	volume of structural layer subregion (m^3)

11.3 Greek Symbols

α	=	total porosity of fuel (dimensionless)
β	=	interconnected porosity of fuel (dimensionless)
β_{fail}	=	interconnected porosity upon failure of cladding (dimensionless) [1]
β_{fr}	=	interconnected porosity of fully frothed fuel (dimensionless) [0.001]
β_{melt}	=	interconnected porosity upon melting of cladding, usually unity (dimensionless) [1]
β_{ox}	=	interconnected porosity upon excessive oxidation of cladding (dimensionless)
β_r	=	interconnected porosity in radial dimension (dimensionless) [1]
β_z	=	interconnected porosity in axial dimension (dimensionless) [1]
β_0	=	initial interconnected porosity of fuel (dimensionless) [0.0001]
$\gamma(i)$	=	activity coefficient of species i (dimensionless)
δ	=	subregion layer thickness (m)
δ_{dep}	=	thickness of a deposited layer (m)

Nomenclature

δ_m	= mass transfer boundary layer thickness (m)
δ_{\max}	= maximum subregion layer thickness (m)
$\delta_{CR}(t)$	= thickness of the alloy film (m) as a function of time t
δ_T	= thermal boundary layer thickness (m)
ΔG	= change in Gibbs free energy ($\text{kg}\cdot\text{m}^2/\text{s}^2\cdot\text{kg}\cdot\text{mol}\cdot\text{K}$)
ε_i	= Lennard-Jones parameter for characteristic energy of self-interaction for species i (dimensionless)
ε_s	= particle-to-particle sticking efficiency (dimensionless)
ε_{PK}	= collision efficiency correction factor due to Prupacher and Klett (dimensionless)
$\zeta(i)$	= the rate of condensation of vapor species i onto an aerosol surface (kg/m^3)
η_b	= deposition efficiency due to flow irregularity (dimensionless)
θ	= vane angle (radians)
$\theta(i)$	= activation temperature of grain lattice diffusion for species i (K)
Θ	= turning angle of a chevron guide (radians)
κ	= permeability (m^2)
κ_r	= radial component of permeability tensor (m^2)
κ_z	= axial component of permeability tensor (m^2)
κ_B	= Boltzmann's constant ($\text{kg}\cdot\text{m}^2/\text{s}^2\cdot\text{K}\cdot\text{molecule}$)
μ	= dynamic viscosity of gas phase ($\text{kg}/\text{m}\cdot\text{s}$)
$\mu(i)$	= dynamic viscosity of pure species i ($\text{kg}/\text{m}\cdot\text{s}$)
ρ	= gas density (kg/m^3)
$\rho(i)$	= density of pure condensed-phase species i (kg/m^3)
ρ_a	= density of an aerosol particle (kg/m^3)
ρ_{dep}	= density of deposited film (kg/m^3)
ρ_S	= density of structure (kg/m^3)
σ^3	= geometric standard deviation (dimensionless)
σ_i	= Lennard-Jones parameter for characteristic diameter of species i (Å)
σ_{ij}	= characteristic diameter for collisions between species i and j (Å)

Nomenclature

$\zeta(i)$	= rate of condensation (evaporation is expressed by a negative value) of vapor species i onto an aerosol surface (kg/m^3)
τ	= scaled time (dimensionless)
ϕ_T	= turbulent energy dissipation rate per unit mass (m^2/s^3)
$\Phi(\omega, m)$	= agglomeration kernel ($\text{m}^3/\text{kg}\cdot\text{s}$), i.e., a measure of the rate at which particles of mass ω coalesce with particles of mass m
$\Phi_B(m, \omega)$	= agglomeration rate of particles of mass m with particles of mass ω due to Brownian diffusion ($\text{m}^3/\text{kg}\cdot\text{s}$)
$\Phi_G(m, \omega)$	= agglomeration rate of particles of mass m with particles of mass ω due to gravitational settling ($\text{m}^3/\text{kg}\cdot\text{s}$)
$\Phi_I(m, \omega)$	= agglomeration rate of particles of mass m with particles of mass ω due to turbulent inertia ($\text{m}^3/\text{kg}\cdot\text{s}$)
$\Phi_S(m, \omega)$	= agglomeration rate of particles of mass m with particles of mass ω due to turbulent shear ($\text{m}^3/\text{kg}\cdot\text{s}$)
ϕ_T	= turbulent energy dissipation rate per unit mass (m^2/s^3)
χ_c	= collisional shape factor (dimensionless) [1]
χ_d	= dynamic shape factor (dimensionless) [1]
ψ	= empirical coefficient for particle diffusion in a laminar flow
ω	= mass of an aerosol particle (kg)
$\Omega_{D, ij}$	= collision integral for mass diffusion in a binary mixture of i and j (dimensionless)
$\Omega_{\mu, i}$	= viscosity collision integral for species i (dimensionless)

11.4 Dimensionless Numbers

Kn	= particle Knudsen number (dimensionless), l_p/r_a
Nu	= Nusselt number (dimensionless), $(HD_H)/k$
Ra	= Rayleigh number (dimensionless), $(g T_s - T_g \rho^2 D_H^3)/(\mu^2 T_s)$
Re	= Reynolds number (dimensionless), $(\rho U D_H)/\mu$
Sc	= Schmidt number (dimensionless), $\mu/\rho D(i)$
Sh	= Sherwood number (dimensionless), D_H/δ_m
St	= Particle Stokes number (dimensionless), $4Cn\rho_a r_a^2 U/9\mu D_H$

11.5 Subscripts

a	= aerosol
b	= bends or flow irregularities
c	= ceiling surface
d	= diffusion
dep	= deposited film
f	= floor surface
fail	= failure point
fr	= fuel frothing
g	= gas or gravitational settling
max	= maximum value
melt	= melting point
o	= offset
r	= radial direction
s	= surface
t	= turbulence
w	= wall surface
z	= axial direction
T	= thermophoresis
C	= control rod surface
G	= fuel grain
F	= fuel pellet or fuel rod surface, depending on whether fuel is clad
I	= insulation
S	= structural surface
O	= initial condition or preexponential coefficient

Nomenclature